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Stephen D. Lowe
(M. S. Thesis)

October 30, 1963

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FRACTIONAL RELEASE OF A TRACER ELEMENT THROUGH A MOVING BOUNDARY

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FRACTIONAL RELEASE OF A TRACER ELEMENT THROUGH A MOVING BOUNDARY

Stephen D. Lowe*

Lawrence Radiation Laboratory
University of California
Berkeley, California

October 30, 1963

ABSTRACT

A full solution for the fractional release of a tracer element through a moving boundary has been obtained for the cases of a slab and a sphere. In both cases, the initial distribution of the tracer is assumed to be uniform throughout the body. For a constant rate of boundary motion, the full solution is valid for all times over the range from zero to complete evaporation of the body, and this solution may be applied to all finite rates of boundary motion.

By applying certain limitations to the time range and to the total amount of boundary motion, the full solutions are reduced to approximate forms that are presented graphically as a family of curves.

For a more limited range of application, i. e., for small values of the quantity $\frac{1}{2}\left(\frac{ba}{D}\right)\left(\frac{Dt}{a^2}\right)^{1/2}$ (< 0.2), where b is the rate of boundary motion, t is the time, D is the diffusion constant, and a is a characteristic dimension of the body (half-width for the slab and radius for the sphere), simplified expressions are developed for the fractional release of the tracer, f, which may be used to more accurately determine the diffusion coefficient, D.

These simplified expressions are

$$f = \frac{2}{\pi^{1/2}}\left(\frac{Dt}{a^2}\right)^{1/2} + \frac{1}{2}\left(\frac{bt}{a}\right) \text{ for the slab,}$$

and

$$f = \frac{6}{\pi^{1/2}}\left(\frac{Dt}{a^2}\right)^{1/2} + \frac{3}{2}\left(\frac{bt}{a}\right) \text{ for the sphere.}$$

---

* Lieutenant, Civil Engineer Corps, United States Navy.

I. INTRODUCTION

A. Basis for the Problem

During his investigation of the diffusion of xenon in uranium monocarbide, Shaked noted the slope of his plot of the fractional release, f vs $(t)^{1/2}$ increased noticeably during a high-temperature anneal.[1] He postulated that evaporation of the uranium monocarbide was responsible for the increase.

A similar increase in the slope of the f vs $(t)^{1/2}$ plot had been reported previously for experiments in the temperature range, 1600 to 2200°C.[2]

With the increasing interest in high-temperature applications for uranium fuels, in thermionics, for example, it is considered of interest to investigate the release of a fission product from the fuel element due to the additional process of evaporation occurring simultaneously with the process of diffusion.

B. Discussion of the Problem

Several investigators have reported diffusion constants for xenon-133 and krypton-85 in uranium dioxide.[3] A lesser number have reported results for the diffusion constant of xenon-133 in uranium monocarbide.[1] In the "conventional" analysis, one assumes a uniform initial concentration of the tracer element in the geometrical body whose boundaries are fixed with time. Evaporation of the body is discussed in a general manner, but the effects are minimized experimentally.[1, 3]

C. Statement of the Problem

This report is an investigation of the effect of evaporation upon the fractional release of a radioactive tracer element from a fuel body. As such, the decay of the tracer is neglected for the purposes of this report (i. e., $\lambda = 0$), although this effect can and should be taken into account for experiments involving long postirradiation anneal time.

An expression for the combined fractional release due to both diffusion and evaporation (i. e., diffusion through a moving boundary) is obtained. This result is compared to the fractional release derived for the case of "pure diffusion" (i. e., diffusion through a stationary boundary).

The analysis is performed for the case of the finite slab and the case of the finite sphere. It is assumed that the initial concentration of the tracer element in the body is uniform and that the concentration of the tracer element at the boundary (moving or stationary) of the body vanishes.

II. THE SLAB PROBLEM

A. Concentration of the Tracer

One seeks a solution for the diffusion equation

$$\frac{\partial C(x,t)}{\partial t} = D\,\frac{\partial^2 C(x,t)}{\partial x^2}\,, \qquad -(a-bt)<x<a-bt \tag{II-1}$$

such that $$C(x,0)=C_0 \tag{II-1a}$$

and $$C[\pm(a-bt),t] = 0 \quad \text{for } 0<t<a/b, \tag{II-1b}$$

where b is the rate of movement of the boundary that may be obtained from kinetic theory if one assumes evaporation in a vacuum of a material of known vapor pressure.[4] The assumption of a constant evaporation rate ignores the possible effect upon vapor pressure, and hence upon the evaporation rate, if there is a change of chemical composition of the solid surface accompanying evaporation. At time $t = a/b$, the sample will have completely sublimed.

Chambré has shown[5] that the solution to Eq. (II-1) that satisfies an initial even function $f(\xi)$ and Eq. (II-1b) may be expressed as

$$C(x,t)=\frac{1}{2(\pi D t)^{1/2}}\left\{\int_{-a}^{a} f(\xi)\exp\left[-\frac{(x-\xi)^2}{4Dt}\right]d\xi + \sum_{n=1}^{\infty}(-1)^n\int_{-a}^{a} f(\xi)\exp\left[\frac{nb}{D}(\xi+na)\right]S(x,t;\xi+2na)\,d\xi\right\}, \tag{II-2}$$

where for the case under study

$$f(\xi)=C_0 \tag{II-2a}$$

and $$S(x,t;\xi)=\exp\left[-\frac{(x-\xi)^2}{4Dt}\right]+\exp\left[-\frac{(x+\xi)^2}{4Dt}\right]. \tag{II-3}$$

Making the substitutions into Eq. (II-2), one obtains the resulting expression for C(x, t):

$$C(x,t)=\frac{C_0}{2(\pi Dt)^{1/2}}\left\{\int_{-a}^{a}\exp\left[-\frac{(x-\xi)^2}{4Dt}\right]d\xi\right.$$
$$\left.+\sum_{n=1}^{\infty}(-1)^n\int_{-a}^{a}\exp\left[\frac{nb}{D}(\xi+na)\right]\left[\exp\left[-\frac{(x-\xi-2na)^2}{4Dt}\right]+\exp\left[-\frac{(x+\xi+2na)^2}{4Dt}\right]\right]d\xi\right\}. \tag{II-4}$$

Performing the integration over ξ (see Appendix D), one may show Eq. (II-4) to be

$$C(x,t)=\frac{C_0}{2}\left\{\operatorname{erf}\left[\frac{x+a}{2(Dt)^{1/2}}\right]-\operatorname{erf}\left[\frac{x-a}{2(Dt)^{1/2}}\right]\right\}$$
$$+\frac{C_0}{2}\sum_{n=1}^{\infty}(-1)^n\exp\left\{-\left[n^2\left(\frac{ba}{D}-\frac{b^2t}{D}\right)\right]\right\}\left\{\exp\left(\frac{nbx}{D}\right)\left[\operatorname{erf}\frac{a(2n+1)-(x+2nbt)}{2(Dt)^{1/2}}\right.\right.$$
$$\left.\left.-\operatorname{erf}\frac{a(2n-1)-(x+2nbt)}{2(Dt)^{1/2}}\right]\right\} \tag{II-5}$$
$$+\frac{C_0}{2}\sum_{n=1}^{\infty}(-1)^n\exp\left\{-\left[n^2\left(\frac{ba}{D}-\frac{b^2t}{D}\right)\right]\right\}\left\{\exp\left(-\frac{nbx}{D}\right)\left[\operatorname{erf}\frac{a(2n+1)+(x-2nbt)}{2(Dt)^{1/2}}\right.\right.$$
$$\left.\left.-\operatorname{erf}\frac{a(2n-1)+(x-2nbt)}{2(Dt)^{1/2}}\right]\right\}.$$

This may be rewritten as

$$C\left(\frac{x}{a},\frac{Dt}{a^2}\right)=\frac{C_0}{2}\left[\operatorname{erf}\frac{1+x/a}{2\left(\frac{Dt}{a^2}\right)^{1/2}}+\operatorname{erf}\frac{1-x/a}{2\left(\frac{Dt}{a^2}\right)^{1/2}}\right]$$
$$+\frac{C_0}{2}\sum_{n=1}^{\infty}(-1)^n\exp\left\{-\left[n^2\left(\frac{ba}{D}-\frac{Dt}{a^2}\frac{b^2a^2}{D^2}\right)\right]\right\}\left\{\exp\left[\frac{nba}{D}\left(\frac{x}{a}\right)\right]\left[\operatorname{erf}\frac{(2n+1)-\left(x/a+2n\frac{Dt}{a^2}\frac{ab}{D}\right)}{2\left(\frac{Dt}{a^2}\right)^{1/2}}\right.\right.$$
$$\left.\left.-\operatorname{erf}\frac{(2n-1)-\left(x/a+2n\frac{Dt}{a^2}\frac{ab}{D}\right)}{2\left(\frac{Dt}{a^2}\right)^{1/2}}\right]\right\} \tag{II-6}$$
$$+\frac{C_0}{2}\sum_{n=1}^{\infty}(-1)^n\exp\left\{-\left[n^2\left(\frac{ba}{D}-\frac{Dt}{a^2}\frac{b^2a^2}{D^2}\right)\right]\right\}\left\{\exp\left[-\frac{nba}{D}\left(\frac{x}{a}\right)\right]\left[\operatorname{erf}\frac{(2n+1)+\left(x/a-2n\frac{Dt}{a^2}\frac{ab}{D}\right)}{2\left(\frac{Dt}{a^2}\right)^{1/2}}\right.\right.$$
$$\left.\left.-\operatorname{erf}\frac{(2n-1)+\left(x/a-2n\frac{Dt}{a^2}\frac{ab}{D}\right)}{2\left(\frac{Dt}{a^2}\right)^{1/2}}\right]\right\}.$$

Making the definitions

$$\tau=\frac{Dt}{a^2} \tag{II-7}$$

and

$$\beta = \frac{ba}{D}, \tag{II-8}$$

where $0 < \beta\tau < 1,$

and substituting into Eq. (II-6), one obtains

$$\begin{aligned} C(x/a,\tau) = {} & \frac{C_0}{2}\left[\operatorname{erf}\left(\frac{1+x/a}{2\tau^{1/2}}\right) + \operatorname{erf}\left(\frac{1-x/a}{2\tau^{1/2}}\right)\right] \\ & + \frac{C_0}{2}\sum_{n=1}^{\infty}(-1)^n \exp\left\{-n\beta\left[n(1-\beta\tau)-x/a\right]\right\}\left\{\operatorname{erf}\frac{2n(1-\beta\tau)+1-x/a}{2\tau^{1/2}}\right. \\ & \qquad \left. - \operatorname{erf}\frac{2n(1-\beta\tau)-1+x/a}{2\tau^{1/2}}\right\} \\ & + \frac{C_0}{2}\sum_{n=1}^{\infty}(-1)^n \exp\left\{-n\beta\left[n(1-\beta\tau)+x/a\right]\right\}\left\{\operatorname{erf}\frac{2n(1-\beta\tau)+1+x/a}{2\tau^{1/2}}\right. \\ & \qquad \left. - \operatorname{erf}\frac{2n(1-\beta\tau)-1+x/a}{2\tau^{1/2}}\right\}. \end{aligned} \tag{II-9}$$

By using Eq. (C-4) and setting B = 0 (i. e., no evaporation or boundary motion), Eq. (II-9) becomes

$$\begin{aligned} C(x/a,\tau) = {} & C_0 - \frac{C_0}{2}\left[\operatorname{erfc}\left(\frac{1+x/a}{2\tau^{1/2}}\right) + \operatorname{erfc}\left(\frac{1-x/a}{2\tau^{1/2}}\right)\right] \\ & - \frac{C_0}{2}\sum_{n=1}^{\infty}(-1)^n\left[\operatorname{erfc}\frac{(2n+1)-x/a}{2\tau^{1/2}} - \operatorname{erfc}\frac{(2n-1)-x/a}{2\tau^{1/2}}\right. \\ & \qquad \left. + \operatorname{erfc}\frac{(2n+1)+x/a}{2\tau^{1/2}} - \operatorname{erfc}\frac{(2n-1)+x/a}{2\tau^{1/2}}\right]. \end{aligned} \tag{II-10}$$

This may be rewritten, after combining terms, as

$$C(x/a,\tau) = C_0 - C_0\sum_{n=0}^{\infty}(-1)^n\left[\operatorname{erfc}\frac{(2n+1)-x/a}{2\tau^{1/2}} + \operatorname{erfc}\frac{(2n+1)+x/a}{2\tau^{1/2}}\right]. \tag{II-11}$$

Equation (II-11) may be recognized as one equivalent to Eq. (A-6), which shows that the expression for the tracer concentration does reduce to that for the stationary boundary case when no evaporation is considered.

B. Total Fractional Release

The total release of the tracer element due to the combined effects of diffusion and evaporation may be obtained by integrating the concentration at any time (τ) across the volume of the slab, dividing the result by the total initial amount of tracer present, and subtracting this quotient from 1. Thus,

$$f = \frac{Q_o - Q(\tau)}{Q_o} = 1 - \frac{Q(\tau)}{Q_o}, \tag{II-12}$$

where

$$Q_o = \frac{1}{a}(2aC_o) \tag{II-12a}$$

and

$$Q(\tau) = \int_{-(1-\beta\tau)}^{(1-\beta\tau)} C(x/a,\tau)\,d(x/a) = 2\int_0^{(1-\beta\tau)} C(x/a,\tau)\,d(x/a)\,. \tag{II-12b}$$

Therefore,

$$\begin{aligned}
f &= 1 - \frac{2\int_0^{(1-\beta\tau)} C(x/a,\tau)\,d(x/a)}{2C_o} \\
&= 1 - \frac{1}{C_o}\int_0^{(1-\beta\tau)} \frac{C_o}{2}\left[\operatorname{erf}\frac{1+x/a}{2\tau^{1/2}} + \operatorname{erf}\frac{1-x/a}{2\tau^{1/2}}\right]d(x/a) \\
&\quad - \frac{1}{C_o}\int_0^{(1-\beta\tau)} \frac{C_o}{2}\sum_{n=1}^{\infty}(-1)^n \exp\left\{-n\beta\left[n(1-\beta\tau)-x/a\right]\right\}\left\{\operatorname{erf}\frac{(2n+1)-(x/a+2n\beta\tau)}{2\tau^{1/2}}\right. \\
&\qquad\qquad \left. - \operatorname{erf}\frac{(2n-1)-(x/a+2n\beta\tau)}{2\tau^{1/2}}\right\}d(x/a) \\
&\quad - \frac{1}{C_o}\int_0^{(1-\beta\tau)} \frac{C_o}{2}\sum_{n=1}^{\infty}(-1)^n \exp\left\{-n\beta\left[n(1-\beta\tau)+x/a\right]\right\}\left\{\operatorname{erf}\frac{(2n+1)+(x/a-2n\beta\tau)}{2\tau^{1/2}}\right. \\
&\qquad\qquad \left. - \operatorname{erf}\frac{(2n-1)+(x/a-2n\beta\tau)}{2\tau^{1/2}}\right\}d(x/a)
\end{aligned}$$

$$= 1 - \frac{1}{2}\int_0^{(1-\beta\tau)}\left[\operatorname{erf}\frac{1+x/a}{2\tau^{1/2}} + \operatorname{erf}\frac{1-x/a}{2\tau^{1/2}}\right]d(x/a) \tag{II-13}$$
$$- \frac{1}{2}\sum_{n=1}^{\infty}(-1)^n \exp\{-n\beta[n(1-\beta\tau)]\}\int_0^{(1-\beta\tau)}\exp[n\beta(x/a)]\left\{\operatorname{erf}\frac{2n(1-\beta\tau)+1-x/a}{2\tau^{1/2}}\right.$$
$$\left. - \operatorname{erf}\frac{2n(1-\beta\tau)-1-x/a}{2\tau^{1/2}}\right\}d(x/a)$$
$$- \frac{1}{2}\sum_{n=1}^{\infty}(-1)^n \exp\{-n\beta[n(1-\beta\tau)]\}\int_0^{(1-\beta\tau)}\exp[-n\beta(x/a)]\left\{\operatorname{erf}\frac{2n(1-\beta\tau)+1+x/a}{2\tau^{1/2}}\right.$$
$$\left. - \operatorname{erf}\frac{2n(1-\beta\tau)-1+x/a}{2\tau^{1/2}}\right\}d(x/a) .$$

Performing the integration and combining, one has

$$f = \beta\tau + \tau^{1/2}\left[\operatorname{ierfc}\frac{\beta\tau}{2\tau^{1/2}} - \operatorname{ierfc}\frac{2-\beta\tau}{2\tau^{1/2}}\right]$$
$$+ \tau^{1/2}\sum_{n,m=1}^{\infty}(-1)^{n+m}\exp[-n\beta(n-1)(1-\beta\tau)]\left[2n\beta\tau^{1/2}\right]^{m-1}\left\{i^m\operatorname{erfc}\frac{(2n-1)(1-\beta\tau)-1}{2\tau^{1/2}}\right.$$
$$\left. - i^m\operatorname{erfc}\frac{(2n-1)(1-\beta\tau)+1}{2\tau^{1/2}}\right\} \tag{II-14}$$
$$+ \tau^{1/2}\sum_{n,m=1}^{\infty}(-1)^{n+m}\exp[-n\beta(n+1)(1-\beta\tau)]\left[2n\beta\tau^{1/2}\right]^{m-1}\left\{i^m\operatorname{erfc}\frac{(2n+1)(1-\beta\tau)+1}{2\tau^{1/2}}\right.$$
$$\left. - i^m\operatorname{erfc}\frac{(2n+1)(1-\beta\tau)-1}{2\tau^{1/2}}\right\} .$$

For $\tau = 0$ $(t = 0)$, the fractional release, given by Eq. (II-14), is zero, as is to be expected; and for $\beta\tau = 1$ (or complete evaporation), the expression becomes

$$f = 1 + \tau^{1/2}\left[\operatorname{ierfc}\frac{1}{2\tau^{1/2}} - \operatorname{ierfc}\frac{1}{2\tau^{1/2}}\right]$$
$$+ \tau^{1/2}\sum_{n,m=1}^{\infty}(-1)^{n+m}\left[\frac{2n}{\tau^{1/2}}\right]^{m-1}\left\{i^m\operatorname{erfc}\frac{-1}{2\tau^{1/2}} - i^m\operatorname{erfc}\frac{1}{2\tau^{1/2}}\right.$$
$$\left. + i^m\operatorname{erfc}\frac{1}{2\tau^{1/2}} - i^m\operatorname{erfc}\frac{-1}{2\tau^{1/2}}\right\},$$

which is equal to 1, after cancellation of equivalent terms, and corresponds to the total release of the tracer.

Setting $\beta = 0$ (no evaporation), Eq. (II-14) becomes

$$f = \frac{1}{\pi^{1/2}}\,\tau^{1/2} - \tau^{1/2}\operatorname{ierfc}\frac{1}{\tau^{1/2}}$$

$$\begin{aligned} &-\tau^{1/2}\sum_{n=1}^{\infty}(-1)^{n}\left\{ i\,\mathrm{erfc}\,\frac{n-1}{\tau^{1/2}} - i\,\mathrm{erfc}\,\frac{n}{\tau^{1/2}}\right\} \\ &-\tau^{1/2}\sum_{n=1}^{\infty}(-1)^{n}\left\{ i\,\mathrm{erfc}\,\frac{n+1}{\tau^{1/2}} - i\,\mathrm{erfc}\,\frac{n}{\tau^{1/2}}\right\}. \end{aligned} \tag{II-15}$$

This may be reduced to

$$f = 2\tau^{1/2}\left[\pi^{-1/2} + 2\sum_{n=1}^{\infty}(-1)^{n}\, i\,\mathrm{erfc}\,\frac{n}{\tau^{1/2}}\right], \tag{II-16}$$

which may be recognized as equivalent to Eq. (A-8), the fractional release under conditions of a stationary boundary.

C. Approximate Expression for the Fractional Release

For the usual values of τ encountered in fission gas-release experiments ($\tau < 0.01$), the expression obtained for the fractional release in Eq. (II-14) may be immediately reduced to

$$\begin{aligned} f = {} & \beta\tau + \tau^{1/2}\, i\,\mathrm{erfc}\,\frac{\beta\tau}{2\tau^{1/2}} \\ & + \tau^{1/2}\sum_{n,m=1}^{\infty}(-1)^{n+m}\exp[-n\beta(n-1)(1-\beta\tau)]\left[2n\beta\tau^{1/2}\right]^{m-1} i^{m}\mathrm{erfc}\,\frac{(2n-1)(1-\beta\tau)-1}{2\tau^{1/2}} \\ & - \tau^{1/2}\sum_{n,m=1}^{\infty}(-1)^{n+m}\exp[-n\beta(n+1)(1-\beta\tau)]\left[2n\beta\tau^{1/2}\right]^{m-1} i^{m}\mathrm{erfc}\,\frac{(2n+1)(1-\beta\tau)-1}{2\tau^{1/2}}. \end{aligned} \tag{II-17}$$

If the further limitation is made that $\beta\tau < 0.5$, Eq. (II-17) may be reduced further to

$$\begin{aligned} f = {} & \beta\tau + \tau^{1/2}\, i\,\mathrm{erfc}\,\frac{\beta\tau}{2\tau^{1/2}} \\ & + \tau^{1/2}\sum_{n,m=1}^{\infty}(-1)^{n+m}\exp[-n\beta(n-1)(1-\beta\tau)]\left[2n\beta\tau^{1/2}\right]^{m-1} i^{m}\mathrm{erfc}\,\frac{(2n-1)(1-\beta\tau)-1}{2\tau^{1/2}}, \end{aligned} \tag{II-18}$$

of which the n = 1 term is of the greatest significance, as follows:

$$f = \beta\tau + \tau^{1/2}\,\mathrm{ierfc}\,\frac{\beta\tau}{2\tau^{1/2}} + \tau^{1/2}\sum_{m=1}^{\infty}(-1)^{m+1}\left[2\beta\tau^{1/2}\right]^{m-1} i^m\mathrm{erfc}\,\frac{-\beta\tau}{2\tau^{1/2}}\,. \qquad \text{(II-19)}$$

By using the relations (C-13) through (C-18), Eq. (II-19) becomes

$$f = \beta\tau + \tau^{1/2}\left[\mathrm{ierfc}\,\frac{\beta\tau^{1/2}}{2} + \sum_{m=1}^{\infty}(4)^{m-1}\left(\frac{\beta\tau^{1/2}}{2}\right)^{m-1} i^m\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2}\right]$$

$$\doteq \beta\tau + 2\tau^{1/2}\,\mathrm{ierfc}\,\frac{\beta\tau^{1/2}}{2} + \tau^{1/2}\sum_{m=1}^{\infty}(4)^m\left(\frac{\beta\tau^{1/2}}{2}\right)^m i^{m+1}\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2}\,. \qquad \text{(II-20)}$$

For large $\frac{\beta\tau^{1/2}}{2}$ (i.e., $\frac{\beta\tau^{1/2}}{2} > 2.5$), Eq. (II-20) reduces to $f = \beta\tau$, which indicates that the release of the tracer is due solely to evaporation.

For $\beta = 0$, Eq. (II-20) becomes

$$f = \frac{2}{\pi^{1/2}}\,\tau^{1/2}, \qquad \text{(II-21)}$$

the approximate expression for fractional release from a slab with stationary boundaries.

Figures II.1 and II.2 show the fractional release from a slab vs $[\mathrm{time}]^{1/2}$ ($\tau^{1/2}$) for various rates of evaporation (β). As a reference, the stationary-boundary plot is given, and in each figure it is the lower line. Figure II.1 is for the longer periods of time, whereas Fig. II.2 represents shorter periods of time.

Figures II.3 and II.4 demonstrate the contribution of the individual terms that make up the expression [Eq. (II-20)] for f. Figure II.3 represents an evaporation rate of $\beta = 10$ for times less than $\tau = 0.01$, and Fig. II.4 covers the time span less than $\tau = 0.0001$ for a higher evaporation rate of $\beta = 50$.

(1) $\beta = 0$ (no evaporation)
(2) $\beta = 2$
(3) $\beta = 10$
(4) $\beta = 20$
(5) $\beta = 50$
(6) $\beta = 100$
(7) $\beta = 200$

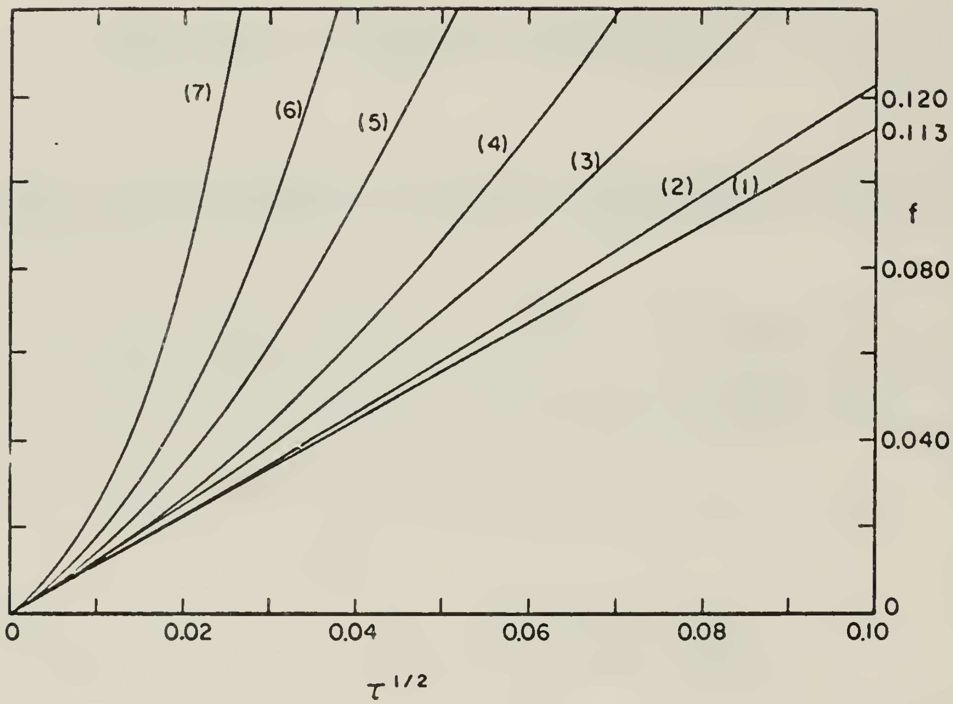

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Fig. II. 1. Fractional release vs $\tau^{1/2}$ for various rates of evaporation.

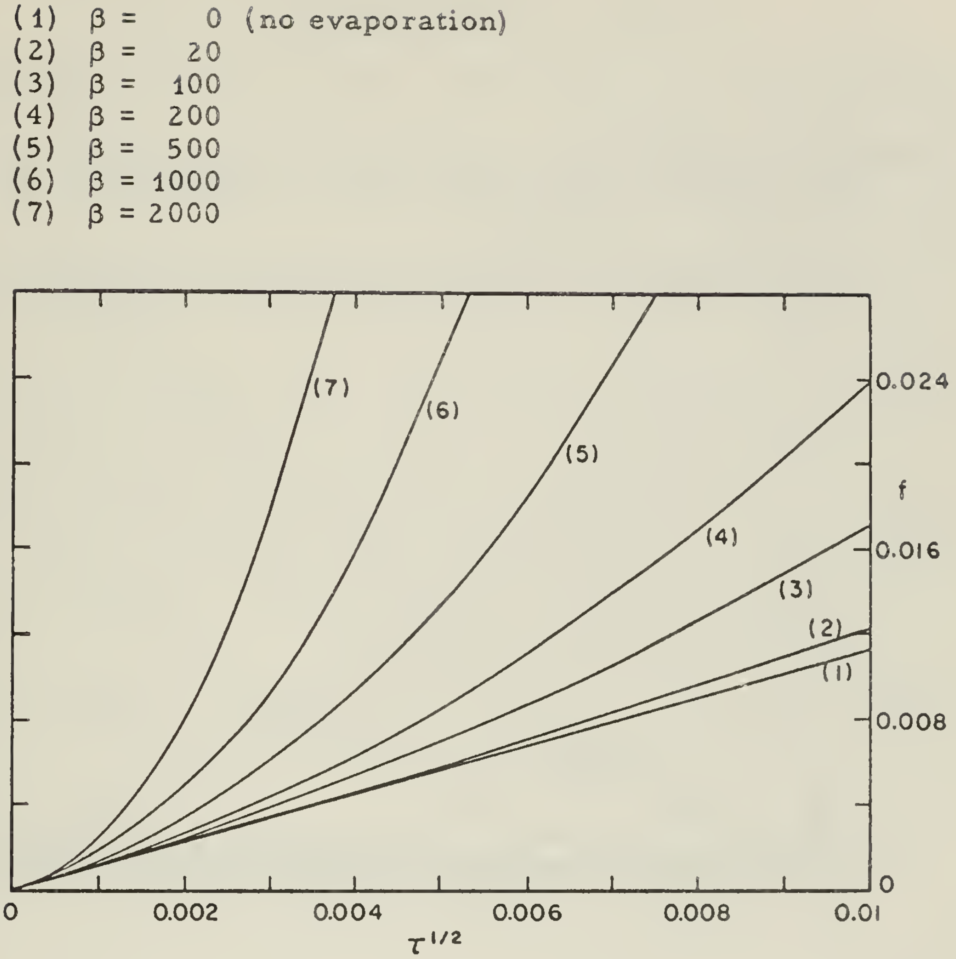

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Fig. II.2. Fractional release vs $\tau^{1/2}$ for various rates of evaporation.

$$f = \beta\tau + 2\tau^{1/2}\,\mathrm{ierfc}\,\frac{\beta\tau^{1/2}}{2} + \tau^{1/2}\sum_{m=1}^{\infty}(4)^m\left(\frac{\beta\tau^{1/2}}{2}\right)^m i^{m+1}\,\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2}$$

— — — Release—no evaporation ($\beta = 0$)
— - — - Combined curve for $\beta = 10$

(1) $\beta\tau$

(2) $2\tau^{1/2}\,\mathrm{ierfc}\,\frac{\beta\tau^{1/2}}{2}$

(3) $\tau^{1/2}(4)\left(\frac{\beta\tau^{1/2}}{2}\right)i^2\,\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2}$

(4) $\tau^{1/2}(4)^2\left(\frac{\beta\tau^{1/2}}{2}\right)^2 i^3\,\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2}$

(5) $\tau^{1/2}(4)^3\left(\frac{\beta\tau^{1/2}}{2}\right)^3 i^4\,\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2}$

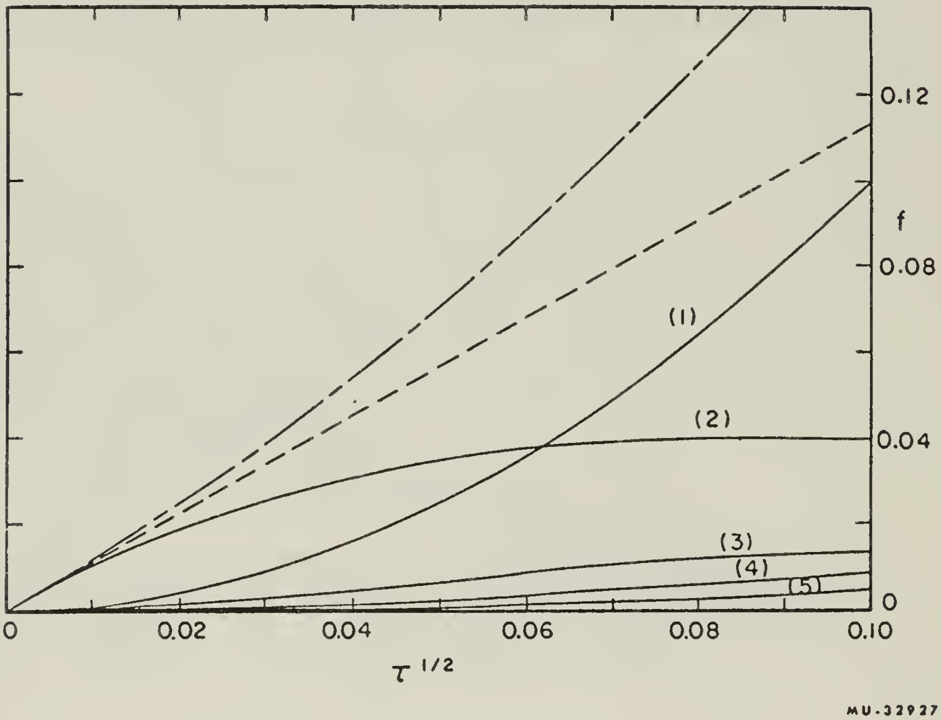

Fig. II. 3. Components of fractional-release curve.

$$f = \beta\tau + 2\tau^{1/2}\,\mathrm{ierfc}\,\frac{\beta\tau^{1/2}}{2} + \tau^{1/2}\sum_{m=1}^{\infty}(4)^m\left(\frac{\beta\tau^{1/2}}{2}\right)^m i^{m+1}\,\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2}$$

— — — Release — no evaporation

— - — - Combined curve for $\beta = 50$

(1) $\beta\tau$

(2) $2\tau^{1/2}\,\mathrm{ierfc}\,\frac{\beta\tau^{1/2}}{2}$

(3) $\tau^{1/2}(4)\left(\frac{\beta\tau^{1/2}}{2}\right)i^2\,\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2}$

(4) $\tau^{1/2}(4)^2\left(\frac{\beta\tau^{1/2}}{2}\right)^2 i^3\,\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2}$

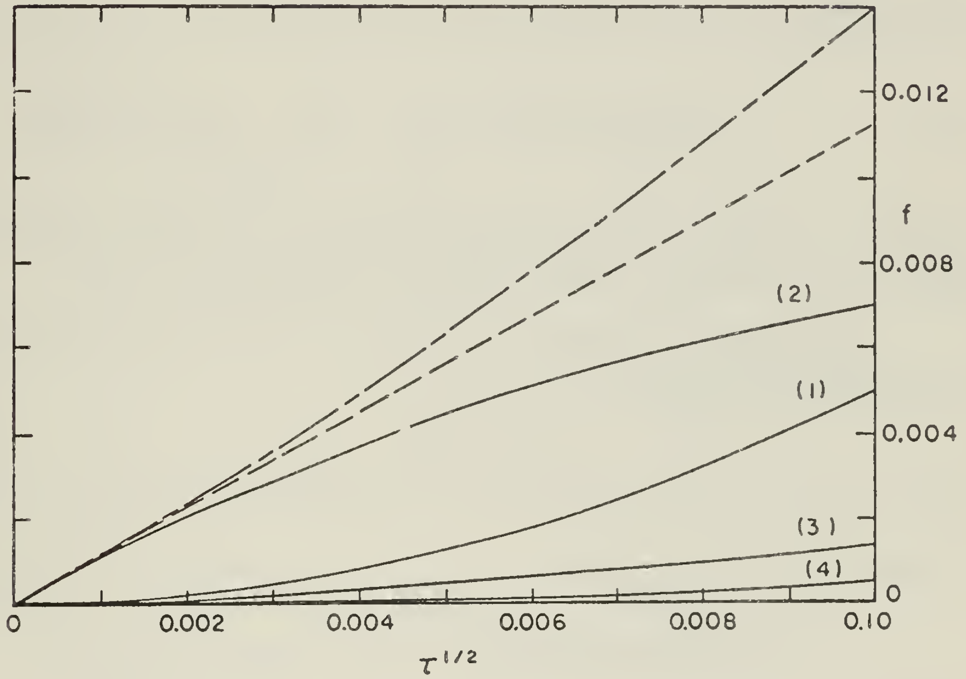

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Fig. II.4. Components of fractional-release curve.

III. THE SPHERE PROBLEM

A. Concentration of the Tracer

A solution for the diffusion equation is sought. Let

$$\frac{\partial C(r,t)}{\partial t} = D\left\{\frac{\partial^2 C(r,t)}{\partial r^2} + \frac{2}{r}\frac{\partial C(r,t)}{\partial r}\right\}, \quad 0<r<a-bt \tag{III-1}$$

such that

$$C(r,0) = C_0 \tag{III-1a}$$

and

$$C(a-bt,t) = 0 \quad \text{for} \quad 0<t<\frac{a}{b}, \tag{III-1b}$$

where b, again, is the rate of boundary movement. At time $t = a/b$, the sample will have been completely sublimed.

Equation (III-1) may be reduced to that for the slab problem by making the substitution

$$u(r,t) = r\,C(r,t), \tag{III-2}$$

subject to the conditions

$$u(r,0) = r\,C_0 \tag{III-2a}$$

and

$$u(a-bt,t) = 0 \quad \text{for} \quad 0<t<\frac{a}{b}\,. \tag{III-2b}$$

Since C(r, t) is finite at interior points, it is necessary to define

$$u(0,t) = 0\,. \tag{III-2c}$$

Chambré[5] has shown the solution of Eq. (III-1), which satisfies an initial even function $f(\xi)$ and Eq. (III-1b), to be

$$\begin{aligned} C(r,t) = \frac{1}{2r(\pi D t)^{1/2}} \Bigg\{ &\int_{-a}^{a} \xi f(\xi) \exp\left[-\frac{(r-\xi)^2}{4Dt}\right] d\xi \\ &+ \sum_{n=1}^{\infty} \int_{-a}^{a} \xi f(\xi) \exp\left[\frac{nb}{D}(\xi+na)\right] S(r,t;\xi+2na)\,d\xi \Bigg\}, \end{aligned} \tag{III-3}$$

where, for this problem

$$f(\xi) = C_0 \tag{III-3a}$$

and $$S(r,t;\xi) = \exp\left[-\frac{(r-\xi)^2}{4Dt}\right] - \exp\left[-\frac{(r+\xi)^2}{4Dt}\right]. \tag{III-4}$$

By making the substitutions into Eq. (III-3), the resulting expression for C(r, t) is

$$\begin{aligned} C(r,t) = \frac{C_0}{2r(\pi D t)^{1/2}} \Bigg\{ & \int_{-a}^{a} \xi \exp\left[-\frac{(r-\xi)^2}{4Dt}\right] d\xi \\ & + \sum_{n=1}^{\infty} \int_{-a}^{a} \xi \exp\left[\frac{nb}{D}(\xi+na)\right]\left[\exp\left(-\frac{(r-\xi-2na)^2}{4Dt}\right)\right. \\ & \qquad \left. - \exp\left(-\frac{(r+\xi+2na)^2}{4Dt}\right)\right] d\xi \Bigg\}. \end{aligned} \tag{III-5}$$

By performing the integration over ξ (see Appendix E), Eq. (III-5) may be shown to be

$$\begin{aligned} C(r,t) = C_0 & - \frac{C_0 a}{2r}\left[\operatorname{erfc}\frac{a-r}{2(Dt)^{1/2}} - \operatorname{erfc}\frac{a+r}{2(Dt)^{1/2}}\right] \\ & - \frac{C_0 a}{2r}\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt-r)\right]\left[\operatorname{erfc}\frac{2n(a-bt)+(a-r)}{2(Dt)^{1/2}}\right. \\ & \qquad \left. + \operatorname{erfc}\frac{2n(a-bt)-(a+r)}{2(Dt)^{1/2}}\right] \\ & + \frac{C_0 a}{2r}\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt+r)\right]\left[\operatorname{erfc}\frac{2n(a-bt)+(a+r)}{2(Dt)^{1/2}}\right. \\ & \qquad \left. + \operatorname{erfc}\frac{2n(a-bt)-(a-r)}{2(Dt)^{1/2}}\right] \\ & - \frac{C_0 a}{r}\left(\frac{Dt}{a^2}\right)^{1/2}\left[\operatorname{ierfc}\frac{a-r}{2(Dt)^{1/2}} - \operatorname{ierfc}\frac{a+r}{2(Dt)^{1/2}}\right] \\ & - \frac{C_0 a}{r}\left(\frac{Dt}{a^2}\right)^{1/2}\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt-r)\right]\left[\operatorname{ierfc}\frac{2n(a-bt)+(a-r)}{2(Dt)^{1/2}}\right. \\ & \qquad \left. - \operatorname{ierfc}\frac{2n(a-bt)-(a+r)}{2(Dt)^{1/2}}\right] \\ & + \frac{C_0 a}{r}\left(\frac{Dt}{a^2}\right)^{1/2}\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt+r)\right]\left[\operatorname{ierfc}\frac{2n(a-bt)+(a+r)}{2(Dt)^{1/2}} - \operatorname{ierfc}\frac{2n(a-bt)-(a-r)}{2(Dt)^{1/2}}\right]. \end{aligned} \tag{III-6}$$

Using the definitions (II-7) and (II-8), then substituting into (III-6), one obtains

$$
\begin{aligned}
C\left(\tfrac{r}{a},\tau\right) = C_0 &- \frac{C_0}{2(r/a)}\left[\operatorname{erfc}\frac{1-r/a}{2\tau^{1/2}} - \operatorname{erfc}\frac{1+r/a}{2\tau^{1/2}}\right] \\
&- \frac{C_0\tau^{1/2}}{r/a}\left[\operatorname{ierfc}\frac{1-r/a}{2\tau^{1/2}} - \operatorname{ierfc}\frac{1+r/a}{2\tau^{1/2}}\right] \\
&- \frac{C_0}{2(r/a)}\sum_{n=1}^{\infty}\exp\left\{-n\beta\left[n(1-\beta\tau)-r/a\right]\right\}\left\{\operatorname{erfc}\frac{2n(1-\beta\tau)+1-r/a}{2\tau^{1/2}}\right. \\
&\qquad\left. + \operatorname{erfc}\frac{2n(1-\beta\tau)-1-r/a}{2\tau^{1/2}}\right\} \\
&+ \frac{C_0}{2(r/a)}\sum_{n=1}^{\infty}\exp\left\{-n\beta\left[n(1-\beta\tau)+r/a\right]\right\}\left\{\operatorname{erfc}\frac{2n(1-\beta\tau)+1+r/a}{2\tau^{1/2}}\right. \\
&\qquad\left. + \operatorname{erfc}\frac{2n(1-\beta\tau)-1+r/a}{2\tau^{1/2}}\right\} \\
&- \frac{C_0\tau^{1/2}}{r/a}\sum_{n=1}^{\infty}\exp\left\{-n\beta\left[n(1-\beta\tau)-r/a\right]\right\}\left\{\operatorname{ierfc}\frac{2n(1-\beta\tau)+1-r/a}{2\tau^{1/2}}\right. \\
&\qquad\left. - \operatorname{ierfc}\frac{2n(1-\beta\tau)-1-r/a}{2\tau^{1/2}}\right\} \\
&+ \frac{C_0\tau^{1/2}}{r/a}\sum_{n=1}^{\infty}\exp\left\{-n\beta\left[n(1-\beta\tau)+r/a\right]\right\}\left\{\operatorname{ierfc}\frac{2n(1-\beta\tau)+1+r/a}{2\tau^{1/2}}\right. \\
&\qquad\left. - \operatorname{ierfc}\frac{2n(1-\beta\tau)-1+r/a}{2\tau^{1/2}}\right\}.
\end{aligned}
\tag{III-7}
$$

Setting $\beta = 0$ (i.e., no evaporation or boundary movement) in Eq. (III-7), it follows that

$$
\begin{aligned}
C\left(\tfrac{r}{a},\tau\right) = C_0 &- \frac{C_0 a}{2r}\left[\operatorname{erfc}\frac{1-r/a}{2\tau^{1/2}} - \operatorname{erfc}\frac{1+r/a}{2\tau^{1/2}}\right] \\
&- \frac{C_0 a}{2r}\sum_{n=1}^{\infty}\left[\operatorname{erfc}\frac{(2n+1)-r/a}{2\tau^{1/2}} + \operatorname{erfc}\frac{(2n-1)-r/a}{2\tau^{1/2}}\right. \\
&\qquad\left. - \operatorname{erfc}\frac{(2n+1)+r/a}{2\tau^{1/2}} - \operatorname{erfc}\frac{(2n-1)+r/a}{2\tau^{1/2}}\right] \\
&- \frac{C_0 a}{r}\tau^{1/2}\left[\operatorname{ierfc}\frac{1-r/a}{2\tau^{1/2}} - \operatorname{ierfc}\frac{1+r/a}{2\tau^{1/2}}\right] \\
&- \frac{C_0 a}{r}\tau^{1/2}\sum_{n=1}^{\infty}\left[\operatorname{ierfc}\frac{(2n+1)-r/a}{2\tau^{1/2}} - \operatorname{ierfc}\frac{(2n-1)-r/a}{2\tau^{1/2}}\right. \\
&\qquad\left. - \operatorname{ierfc}\frac{(2n+1)+r/a}{2\tau^{1/2}} + \operatorname{ierfc}\frac{(2n-1)+r/a}{2\tau^{1/2}}\right].
\end{aligned}
\tag{III-8}
$$

The ierfc terms reduce to zero, and after some recombination, Eq. (III-8) becomes

$$C\left(\frac{r}{a},\tau\right) = C_0 - \frac{C_0 a}{r}\sum_{n=0}^{\infty}\left[\operatorname{erfc}\frac{(2n+1)-r/a}{2\tau^{1/2}} - \operatorname{erfc}\frac{(2n+1)+r/a}{2\tau^{1/2}}\right] \tag{III-9}$$

This may be recognized as equivalent to Eq. (B-6), which shows the expression for the tracer concentration to reduce to that for the stationary-boundary case when no evaporation is considered.

B. Total Fractional Release

The total release of the tracer element due to the combined effects of diffusion and evaporation may be obtained by integrating the concentration at any time (τ) throughout the volume of the sphere, dividing this result by the total initial amount of tracer present, and subtracting this quotient from 1. Hence,

$$f = \frac{Q_0 - Q(\tau)}{Q_0} = 1 - \frac{Q(\tau)}{Q_0}, \tag{III-10}$$

where $$Q_0 = \frac{1}{a^3}\left(\frac{4}{3}\pi a^3 C_0\right) \tag{III-10a}$$

and $$Q(\tau) = \int_0^{(1-\beta\tau)} 4\pi (r/a)^2 C(r/a,\tau)\, d(r/a). \tag{III-10b}$$

Thus,

$$\begin{aligned} f &= 1 - \frac{4\pi\int_0^{(1-\beta\tau)} (r/a)^2 C(r/a,\tau)\, d(r/a)}{4/3\ \pi C_0} \\ &= 1 - \frac{3}{C_0}\int_0^{(1-\beta\tau)} (r/a)^2 C_0\, d(r/a) + \frac{3}{C_0}\int_0^{(1-\beta\tau)} (r/a)^2 \frac{C_0}{2(r/a)}\left[\operatorname{erfc}\frac{1-r/a}{2\tau^{1/2}}\right. \\ &\qquad\left. - \operatorname{erfc}\frac{1+r/a}{2\tau^{1/2}}\right] d(r/a) \\ &\quad + \frac{3}{C_0}\int_0^{(1-\beta\tau)} (r/a)^2 \frac{C_0}{2(r/a)} \sum_{n=1}^{\infty} \exp\left\{-n\beta\left[n(1-\beta\tau)-r/a\right]\right\}\left\{\operatorname{erfc}\frac{2n(1-\beta\tau)+1-r/a}{2\tau^{1/2}}\right. \\ &\qquad\left. + \operatorname{erfc}\frac{2n(1-\beta\tau)-1-r/a}{2\tau^{1/2}}\right\} d(r/a) \end{aligned}$$

$$
\begin{aligned}
&-\frac{3}{C_0}\int_0^{(1-\beta\tau)}(r/a)^2\frac{C_0}{2(r/a)}\sum_{n=1}^{\infty}\exp\left\{-n\beta\left[n(1-\beta\tau)+r/a\right]\right\}\left\{\operatorname{erfc}\frac{2n(1-\beta\tau)+1+r/a}{2\tau^{1/2}}\right.\\
&\qquad\qquad\left.+\operatorname{erfc}\frac{2n(1-\beta\tau)-1+r/a}{2\tau^{1/2}}\right\}d(r/a)\\
&+\frac{3}{C_0}\int_0^{(1-\beta\tau)}(r/a)^2\frac{C_0\tau^{1/2}}{(r/a)}\left[\operatorname{ierfc}\frac{1-r/a}{2\tau^{1/2}}-\operatorname{ierfc}\frac{1+r/a}{2\tau^{1/2}}\right]d(r/a)\\
&+\frac{3}{C_0}\int_0^{1-\beta\tau}(r/a)^2\frac{C_0\tau^{1/2}}{(r/a)}\sum_{n=1}^{\infty}\exp\left\{-n\beta\left[n(1-\beta\tau)-r/a\right]\right\}\left\{\operatorname{ierfc}\frac{2n(1-\beta\tau)+1-r/a}{2\tau^{1/2}}\right.\\
&\qquad\qquad\left.-\operatorname{ierfc}\frac{2n(1-\beta\tau)-1-r/a}{2\tau^{1/2}}\right\}d(r/a)\\
&-\frac{3}{C_0}\int_0^{(1-\beta\tau)}(r/a)^2\frac{C_0\tau^{1/2}}{(r/a)}\sum_{n=1}^{\infty}\exp\left\{-n\beta\left[n(1-\beta\tau)+r/a\right]\right\}\left\{\operatorname{ierfc}\frac{2n(1-\beta\tau)+1+r/a}{2\tau^{1/2}}\right.\\
&\qquad\qquad\left.-\operatorname{ierfc}\frac{2n(1-\beta\tau)-1+r/a}{2\tau^{1/2}}\right\}d(r/a)\\
&=1-3\int_0^{(1-\beta\tau)}(r/a)^2d(r/a)+\frac{3}{2}\int_0^{(1-\beta\tau)}(r/a)\left[\operatorname{erfc}\frac{1-r/a}{2\tau^{1/2}}-\operatorname{erfc}\frac{1+r/a}{2\tau^{1/2}}\right]d(r/a)\\
&\quad+\frac{3}{2}\int_0^{(1-\beta\tau)}(r/a)\sum_{n=1}^{\infty}\exp\left\{-n\beta\left[n(1-\beta\tau)-r/a\right]\right\}\left\{\operatorname{erfc}\frac{2n(1-\beta\tau)+1-r/a}{2\tau^{1/2}}\right.\\
&\qquad\qquad\left.+\operatorname{erfc}\frac{2n(1-\beta\tau)-1-r/a}{2\tau^{1/2}}\right\}d(r/a)\\
&\quad-\frac{3}{2}\int_0^{(1-\beta\tau)}(r/a)\sum_{n=1}^{\infty}\exp\left\{-n\beta\left[n(1-\beta\tau)+r/a\right]\right\}\left\{\operatorname{erfc}\frac{2n(1-\beta\tau)+1+r/a}{2\tau^{1/2}}\right.\\
&\qquad\qquad\left.+\operatorname{erfc}\frac{2n(1-\beta\tau)-1+r/a}{2\tau^{1/2}}\right\}d(r/a)\\
&\quad+3\tau^{1/2}\int_0^{(1-\beta\tau)}(r/a)\left[\operatorname{ierfc}\frac{1-r/a}{2\tau^{1/2}}-\operatorname{ierfc}\frac{1+r/a}{2\tau^{1/2}}\right]d(r/a)\\
&\quad+3\tau^{1/2}\int_0^{(1-\beta\tau)}(r/a)\sum_{n=1}^{\infty}\exp\left\{-n\beta\left[n(1-\beta\tau)-r/a\right]\right\}\left\{\operatorname{ierfc}\frac{2n(1-\beta\tau)+1-r/a}{2\tau^{1/2}}\right.\\
&\qquad\qquad\left.-\operatorname{ierfc}\frac{2n(1-\beta\tau)-1-r/a}{2\tau^{1/2}}\right\}d(r/a)\\
&\quad-3\tau^{1/2}\int_0^{(1-\beta\tau)}(r/a)\sum_{n=1}^{\infty}\exp\left\{-n\beta\left[n(1-\beta\tau)+r/a\right]\right\}\left\{\operatorname{ierfc}\frac{2n(1-\beta\tau)+1+r/a}{2\tau^{1/2}}\right.\\
&\qquad\qquad\left.-\operatorname{ierfc}\frac{2n(1-\beta\tau)-1+r/a}{2\tau^{1/2}}\right\}d(r/a).
\end{aligned}
\tag{III-11}
$$

Integrating and combining the terms in (III-11), one finds

$$
\begin{aligned}
f = {} & 3\beta\tau - 3(\beta\tau)^2 + (\beta\tau)^3 + 3\tau^{1/2}(1-\beta\tau)\left(i\,\mathrm{erfc}\,\frac{\beta\tau}{2\tau^{1/2}} + i\,\mathrm{erfc}\,\frac{2-\beta\tau}{2\tau^{1/2}}\right) \\
& - 6\tau\left(i^2\mathrm{erfc}\,\frac{\beta\tau}{2\tau^{1/2}} - i^2\mathrm{erfc}\,\frac{2-\beta\tau}{2\tau^{1/2}}\right) + 6\tau(1-\beta\tau)\left(i^2\mathrm{erfc}\,\frac{\beta\tau}{2\tau^{1/2}} + i^2\mathrm{erfc}\,\frac{2-\beta\tau}{2\tau^{1/2}}\right) \\
& - 12\tau^{3/2}\left(i^3\mathrm{erfc}\,\frac{\beta\tau}{2\tau^{1/2}} - i^3\mathrm{erfc}\,\frac{2-\beta\tau}{2\tau^{1/2}}\right) \\
& + 3\tau^{1/2}(1-\beta\tau)\sum_{n,m=1}^{\infty}(-1)^{m+1}(2n\beta\tau^{1/2})^{m-1}\exp\left[-n\beta(n-1)(1-\beta\tau)\right]\left[i^m\mathrm{erfc}\,\frac{(2n-1)(1-\beta\tau)+1}{2\tau^{1/2}}\right. \\
& \qquad\qquad \left. + i^m\mathrm{erfc}\,\frac{(2n-1)(1-\beta\tau)-1}{2\tau^{1/2}}\right] \\
& + 3\tau^{1/2}(1-\beta\tau)\sum_{n,m=1}^{\infty}(-1)^{m+1}(2n\beta\tau^{1/2})^{m-1}\exp\left[-n\beta(n+1)(1-\beta\tau)\right]\left[i^m\mathrm{erfc}\,\frac{(2n+1)(1-\beta\tau)+1}{2\tau^{1/2}}\right. \\
& \qquad\qquad \left. + i^m\mathrm{erfc}\,\frac{(2n+1)(1-\beta\tau)-1}{2\tau^{1/2}}\right] \\
& + 6\tau\sum_{\substack{n=1\\m=2}}^{\infty}(-1)^{m+1}(m-1)(2n\beta\tau^{1/2})^{m-2}\exp\left[-n\beta(n-1)(1-\beta\tau)\right]\left[i^m\mathrm{erfc}\,\frac{(2n-1)(1-\beta\tau)+1}{2\tau^{1/2}}\right. \\
& \qquad\qquad \left. + i^m\mathrm{erfc}\,\frac{(2n-1)(1-\beta\tau)-1}{2\tau^{1/2}}\right] \\
& - 6\tau\sum_{\substack{n=1\\m=2}}^{\infty}(-1)^{m+1}(m-1)(2n\beta\tau^{1/2})^{m-2}\exp\left[-n\beta(n+1)(1-\beta\tau)\right]\left[i^m\mathrm{erfc}\,\frac{(2n+1)(1-\beta\tau)+1}{2\tau^{1/2}}\right. \\
& \qquad\qquad \left. + i^m\mathrm{erfc}\,\frac{(2n+1)(1-\beta\tau)-1}{2\tau^{1/2}}\right] \\
& + 6\tau(1-\beta\tau)\sum_{\substack{n=1\\m=2}}^{\infty}(-1)^{m}(2n\beta\tau^{1/2})^{m-2}\exp\left[-n\beta(n-1)(1-\beta\tau)\right]\left[i^m\mathrm{erfc}\,\frac{(2n-1)(1-\beta\tau)+1}{2\tau^{1/2}}\right. \\
& \qquad\qquad \left. - i^m\mathrm{erfc}\,\frac{(2n-1)(1-\beta\tau)-1}{2\tau^{1/2}}\right] \\
& + 6\tau(1-\beta\tau)\sum_{\substack{n=1\\m=2}}^{\infty}(-1)^{m}(2n\beta\tau^{1/2})^{m-2}\exp\left[-n\beta(n+1)(1-\beta\tau)\right]\left[i^m\mathrm{erfc}\,\frac{(2n+1)(1-\beta\tau)+1}{2\tau^{1/2}}\right. \\
& \qquad\qquad \left. - i^m\mathrm{erfc}\,\frac{(2n+1)(1-\beta\tau)-1}{2\tau^{1/2}}\right] \\
& + 12\tau^{3/2}\sum_{\substack{n=1\\m=3}}^{\infty}(-1)^{m}(m-2)(2n\beta\tau^{1/2})^{m-3}\exp\left[-n\beta(n-1)(1-\beta\tau)\right]\left[i^m\mathrm{erfc}\,\frac{(2n-1)(1-\beta\tau)+1}{2\tau^{1/2}}\right. \\
& \qquad\qquad \left. - i^m\mathrm{erfc}\,\frac{(2n-1)(1-\beta\tau)-1}{2\tau^{1/2}}\right] \\
& - 12\tau^{3/2}\sum_{\substack{n=1\\m=3}}^{\infty}(-1)^{m}(m-2)(2n\beta\tau^{1/2})^{m-3}\exp\left[-n\beta(n+1)(1-\beta\tau)\right]\left[i^m\mathrm{erfc}\,\frac{(2n+1)(1-\beta\tau)+1}{2\tau^{1/2}}\right. \\
& \qquad\qquad \left. - i^m\mathrm{erfc}\,\frac{(2n+1)(1-\beta\tau)-1}{2\tau^{1/2}}\right].
\end{aligned}
\tag{III-12}
$$

For $\tau = 0$ ($t = 0$), the fractional release, as given by Eq. (III-12), is zero, as expected; and for $\beta\tau = 1$ (or complete evaporation), the expression becomes

$$\begin{aligned} f = {} & 3 - 3 + 1 - 6\tau\left(i^2\mathrm{erfc}\,\frac{1}{2\tau^{1/2}} - i^2\mathrm{erfc}\,\frac{1}{2\tau^{1/2}}\right) \\ & - 12\tau^{3/2}\left(i^3\mathrm{erfc}\,\frac{1}{2\tau^{1/2}} - i^3\mathrm{erfc}\,\frac{1}{2\tau^{1/2}}\right) \\ & + 6\tau\sum_{\substack{n=1\\m=2}}^{\infty}(-1)^{m+1}(m-1)\left(\frac{2n}{\tau^{1/2}}\right)^{m-2}\left(i^m\mathrm{erfc}\,\frac{1}{2\tau^{1/2}} + i^m\mathrm{erfc}\,\frac{-1}{2\tau^{1/2}}\right. \\ & \qquad \left. - i^m\mathrm{erfc}\,\frac{1}{2\tau^{1/2}} - i^m\mathrm{erfc}\,\frac{-1}{2\tau^{1/2}}\right) \\ & + 12\tau^{3/2}\sum_{\substack{n=1\\m=3}}^{\infty}(-1)^{m}(m-2)\left(\frac{2n}{\tau^{1/2}}\right)^{m-3}\left(i^m\mathrm{erfc}\,\frac{1}{2\tau^{1/2}} - i^m\mathrm{erfc}\,\frac{-1}{2\tau^{1/2}}\right. \\ & \qquad \left. - i^m\mathrm{erfc}\,\frac{1}{2\tau^{1/2}} + i^m\mathrm{erfc}\,\frac{-1}{2\tau^{1/2}}\right), \end{aligned}$$

which is equal to 1, after cancellation of equivalent terms, and corresponds to total release of the tracer.

Setting $\beta = 0$ (no evaporation), Eq. (III-12) becomes

$$\begin{aligned} f = {} & \frac{3}{\pi^{1/2}}\tau^{1/2} + 3\tau^{1/2}\,i\mathrm{erfc}\,\frac{1}{\tau^{1/2}} - \frac{3}{2}\tau + 6\tau\, i^2\mathrm{erfc}\,\frac{1}{\tau^{1/2}} + \frac{3}{2}\tau \\ & + 6\tau\, i^2\mathrm{erfc}\,\frac{1}{\tau^{1/2}} - 12\tau^{3/2}\left(\frac{1}{6}\pi^{-1/2}\right) + 12\tau^{3/2}\, i^3\mathrm{erfc}\,\frac{1}{\tau^{1/2}} \\ & + 3\tau^{1/2}\sum_{n=1}^{\infty}\left\{i\mathrm{erfc}\,\frac{n}{\tau^{1/2}} + i\mathrm{erfc}\,\frac{n-1}{\tau^{1/2}} + i\mathrm{erfc}\,\frac{n+1}{\tau^{1/2}} + i\mathrm{erfc}\,\frac{n}{\tau^{1/2}}\right\} \\ & + 6\tau\sum_{n=1}^{\infty}\left\{i^2\mathrm{erfc}\,\frac{n+1}{\tau^{1/2}} + i^2\mathrm{erfc}\,\frac{n}{\tau^{1/2}}\right. \\ & \qquad \left. - i^2\mathrm{erfc}\,\frac{n}{\tau^{1/2}} - i^2\mathrm{erfc}\,\frac{n-1}{\tau^{1/2}}\right\} \\ & + 6\tau\sum_{n=1}^{\infty}\left\{i^2\mathrm{erfc}\,\frac{n}{\tau^{1/2}} - i^2\mathrm{erfc}\,\frac{n-1}{\tau^{1/2}} + i^2\mathrm{erfc}\,\frac{n+1}{\tau^{1/2}} - i^2\mathrm{erfc}\,\frac{n}{\tau^{1/2}}\right\} \\ & - 12\tau^{3/2}\sum_{n=1}^{\infty}\left\{i^3\mathrm{erfc}\,\frac{n}{\tau^{1/2}} - i^3\mathrm{erfc}\,\frac{n-1}{\tau^{1/2}} - i^3\mathrm{erfc}\,\frac{n+1}{\tau^{1/2}} + i^3\mathrm{erfc}\,\frac{n}{\tau^{1/2}}\right\}. \end{aligned} \tag{III-13}$$

This may be reduced to

$$f = 6\tau^{1/2}\left[\pi^{-1/2} + 2\sum_{n=1}^{\infty} i\mathrm{erfc}\,\frac{n}{\tau^{1/2}}\right] - 3\tau, \tag{III-14}$$

which may be recognized as equivalent to Eq. (B-8), the fractional release under conditions of a stationary boundary.

C. Approximate Expression for the Fractional Release

For the usual values of τ encountered in fission-gas-release experiments ($\tau < 0.01$), the expression obtained for the fractional release in Eq. (III-12) may be immediately reduced to

$$\begin{aligned}
f = {} & 3\beta\tau - 3(\beta\tau)^2 + (\beta\tau)^3 + 3\tau^{1/2}(1-\beta\tau)\, i\,\mathrm{erfc}\, \frac{\beta\tau}{2\tau^{1/2}} - 6\tau\, i^2\mathrm{erfc}\, \frac{\beta\tau}{2\tau^{1/2}} \\
& + 6\tau(1-\beta\tau)\, i^2\mathrm{erfc}\, \frac{\beta\tau}{2\tau^{1/2}} - 12\tau^{3/2}\, i^3\mathrm{erfc}\, \frac{\beta\tau}{2\tau^{1/2}} \\
& + 3\tau^{1/2}(1-\beta\tau) \sum_{n,m=1}^{\infty} (-1)^{m+1} (2n\beta\tau^{1/2})^{m-1} \Big\{ \exp[-n\beta(n-1)(1-\beta\tau)]\, i^m\mathrm{erfc}\, \frac{(2n-1)(1-\beta\tau)-1}{2\tau^{1/2}} \\
& \qquad + \exp[-n\beta(n+1)(1-\beta\tau)]\, i^m\mathrm{erfc}\, \frac{(2n+1)(1-\beta\tau)-1}{2\tau^{1/2}} \Big\} \\
& + 6\tau \sum_{\substack{n=1\\m=2}}^{\infty} (-1)^{m+1} (m-1)(2n\beta\tau^{1/2})^{m-2} \Big\{ \exp[-n\beta(n-1)(1-\beta\tau)]\, i^m\mathrm{erfc}\, \frac{(2n-1)(1-\beta\tau)-1}{2\tau^{1/2}} \\
& \qquad - \exp[-n\beta(n+1)(1-\beta\tau)]\, i^m\mathrm{erfc}\, \frac{(2n+1)(1-\beta\tau)-1}{2\tau^{1/2}} \Big\} \\
& - 6\tau(1-\beta\tau) \sum_{\substack{n=1\\m=2}}^{\infty} (-1)^{m} (2n\beta\tau^{1/2})^{m-2} \Big\{ \exp[-n\beta(n-1)(1-\beta\tau)]\, i^m\mathrm{erfc}\, \frac{(2n-1)(1-\beta\tau)-1}{2\tau^{1/2}} \\
& \qquad + \exp[-n\beta(n+1)(1-\beta\tau)]\, i^m\mathrm{erfc}\, \frac{(2n+1)(1-\beta\tau)-1}{2\tau^{1/2}} \Big\} \\
& - 12\tau^{3/2} \sum_{\substack{n=1\\m=3}}^{\infty} (-1)^{m} (m-2)(2n\beta\tau^{1/2})^{m-3} \Big\{ \exp[-n\beta(n-1)(1-\beta\tau)]\, i^m\mathrm{erfc}\, \frac{(2n+1)(1-\beta\tau)-1}{2\tau^{1/2}} \\
& \qquad - \exp[-n\beta(n+1)(1-\beta\tau)]\, i^m\mathrm{erfc}\, \frac{(2n+1)(1-\beta\tau)-1}{2\tau^{1/2}} \Big\}.
\end{aligned} \tag{III-15}$$

By making the further limitation that $\beta\tau < 0.5$, one obtains

$$\begin{aligned}
f = {} & 3\beta\tau - 3(\beta\tau)^2 + (\beta\tau)^3 + 3\tau^{1/2}(1-\beta\tau)\, i\,\mathrm{erfc}\, \frac{\beta\tau}{2\tau^{1/2}} \\
& - 6\tau\, i^2\mathrm{erfc}\, \frac{\beta\tau}{2\tau^{1/2}} + 6\tau(1-\beta\tau)\, i^2\mathrm{erfc}\, \frac{\beta\tau}{2\tau^{1/2}} \\
& - 12\tau^{3/2}\, i^3\mathrm{erfc}\, \frac{\beta\tau}{2\tau^{1/2}} \\
& + 3\tau^{1/2}(1-\beta\tau) \sum_{n,m=1}^{\infty} (-1)^{m+1} (2n\beta\tau^{1/2})^{m-1} \exp[-n\beta(n-1)(1-\beta\tau)]\, i^m\mathrm{erfc}\, \frac{(2n-1)(1-\beta\tau)-1}{2\tau^{1/2}}
\end{aligned}$$

$$\begin{aligned}
&+6\tau\sum_{\substack{n=1\\m=2}}^{\infty}(-1)^{m+1}(m-1)(2n\beta\tau^{1/2})^{m-2}\exp[-n\beta(n-1)(1-\beta\tau)]\, i^m\operatorname{erfc}\frac{(2n-1)(1-\beta\tau)-1}{2\tau^{1/2}}\\
&-6\tau(1-\beta\tau)\sum_{\substack{n=1\\m=2}}^{\infty}(-1)^{m}(2n\beta\tau^{1/2})^{m-2}\exp[-n\beta(n-1)(1-\beta\tau)]\, i^m\operatorname{erfc}\frac{(2n-1)(1-\beta\tau)-1}{2\tau^{1/2}}\\
&-12\tau^{3/2}\sum_{\substack{n=1\\m=3}}^{\infty}(-1)^{m}(m-2)(2n\beta\tau^{1/2})^{m-3}\exp[-n\beta(n-1)(1-\beta\tau)]\, i^m\operatorname{erfc}\frac{(2n-1)(1-\beta\tau)-1}{2\tau^{1/2}}\,,
\end{aligned}\tag{III-16}$$

of which the n = 1 term is of the greatest significance, as follows:

$$\begin{aligned}
f = {}&3\beta\tau-3(\beta\tau)^2+(\beta\tau)^3+3\tau^{1/2}(1-\beta\tau)\, i\operatorname{erfc}\frac{\beta\tau}{2\tau^{1/2}}\\
&-6\tau\, i^2\operatorname{erfc}\frac{\beta\tau}{2\tau^{1/2}}+6\tau(1-\beta\tau)\, i^2\operatorname{erfc}\frac{\beta\tau}{2\tau^{1/2}}\\
&-12\tau^{3/2}\, i^3\operatorname{erfc}\frac{\beta\tau}{2\tau^{1/2}}\\
&+3\tau^{1/2}(1-\beta\tau)\sum_{m=1}^{\infty}(-1)^{m+1}(2\beta\tau^{1/2})^{m-1}\, i^m\operatorname{erfc}\frac{-\beta\tau}{2\tau^{1/2}}\\
&+6\tau\sum_{m=2}^{\infty}(-1)^{m+1}(m-1)(2\beta\tau^{1/2})^{m-2}\, i^m\operatorname{erfc}\frac{-\beta\tau}{2\tau^{1/2}}\\
&-6\tau(1-\beta\tau)\sum_{m=2}^{\infty}(-1)^{m}(2\beta\tau^{1/2})^{m-2}\, i^m\operatorname{erfc}\frac{-\beta\tau}{2\tau^{1/2}}\\
&-12\tau^{3/2}\sum_{m=3}^{\infty}(-1)^{m}(m-2)(2\beta\tau^{1/2})^{m-3}\, i^m\operatorname{erfc}\frac{-\beta\tau}{2\tau^{1/2}}\,.
\end{aligned}\tag{III-17}$$

By using the relations (C-13) through (C-19), Eq. (III-17) becomes

$$\begin{aligned}
f = {}&3\beta\tau(1-\beta\tau)+(\beta\tau)^3-3\tau-3\tau(1-\beta\tau)\\
&+6\tau^{1/2}(1-\beta\tau)\, i\operatorname{erfc}\frac{\beta\tau^{1/2}}{2}+12\tau(1-\beta\tau)\, i^2\operatorname{erfc}\frac{\beta\tau^{1/2}}{2}
\end{aligned}$$

$$+3\tau^{1/2}(1-\beta\tau)\sum_{m=1}^{\infty}(4)^m\left(\frac{\beta\tau^{1/2}}{2}\right)^m i^{m+1}\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2}$$

$$+6\tau(1-\beta\tau)\sum_{m=1}^{\infty}(4)^m\left(\frac{\beta\tau^{1/2}}{2}\right)^m i^{m+2}\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2} \qquad \text{(III-18)}$$

$$+6\tau\sum_{m=1}^{\infty}(m+1)(4)^m\left(\frac{\beta\tau^{1/2}}{2}\right)^m i^{m+2}\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2}$$

$$+12\tau^{3/2}\sum_{m=1}^{\infty}(m+1)(4)^m\left(\frac{\beta\tau^{1/2}}{2}\right)^m i^{m+3}\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2}\,.$$

The last three summations will be small compared to the first terms; therefore, f will be approximated by

$$f=3\beta\tau(1-\beta\tau)+(\beta\tau)^3-3\tau-3\tau(1-\beta\tau)+12\tau(1-\beta\tau)\,i^2\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2}$$

$$+3\tau^{1/2}(1-\beta\tau)\left[2\,i\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2}+\sum_{m=1}^{\infty}(4)^m\left(\frac{\beta\tau^{1/2}}{2}\right)^m i^{m+1}\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2}\right]. \qquad \text{(III-19)}$$

For large $\frac{\beta\tau^{1/2}}{2}$ (i.e., $\frac{\beta\tau^{1/2}}{2} > 2.5$), Eq. (III-19) will reduce to

$$f=3\beta\tau(1-\beta\tau)+(\beta\tau)^3-3\tau-3\tau(1-\beta\tau),$$

which indicates that the release of the tracer is due primarily to evaporation.

For $\beta=0$, Eq. (III-19) becomes

$$f=\frac{6}{\pi^{1/2}}\tau^{1/2}-3\tau, \qquad \text{(III-20)}$$

the approximate expression for fractional release from a sphere whose boundaries are stationary.

If a further restriction is made, such that $\tau^{1/2} < 0.01$ (or $\tau < 0.0001$), then those terms in Eq. (III-19) having τ as a coefficient (excepting $\beta\tau$ terms) may be neglected, and one obtains

$$\begin{aligned} f = {} & 3\beta\tau(1-\beta\tau)+(\beta\tau)^3 \\ & +3\tau^{1/2}(1-\beta\tau)\left[2\,\mathrm{ierfc}\,\frac{\beta\tau^{1/2}}{2}+\sum_{m=1}^{\infty}(4)^m\left(\frac{\beta\tau^{1/2}}{2}\right)^m i^{m+1}\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2}\right]. \end{aligned} \qquad \text{(III-21)}$$

For large $\frac{\beta\tau^{1/2}}{2}$, Eq. (III-21) reduces to

$$f = 3\beta\tau(1-\beta\tau)+(\beta\tau)^3,$$

which indicates the release of the tracer to be due solely to evaporation.

For $\beta = 0$, Eq. (III-21) becomes

$$f = \frac{6}{\pi^{1/2}}\tau^{1/2}, \qquad \text{(III-22)}$$

the more familiar expression for fractional release from a sphere with stationary boundaries.

Figures III.1 and III.2 display the fractional release from a sphere vs [time]$^{1/2}$ ($\tau^{1/2}$) for various rates of evaporation (β). As a reference, the release for the case of a stationary boundary ($\beta = 0$) is given for each figure; see line (1). Figure III.1 (note the dotted line) in addition, shows the effect of neglecting the 3τ term in Eq. (III-20) for longer periods of time. Figure III.2 represents the release of the tracer element for shorter time periods.

— — — $f = \frac{6}{\pi^{1/2}} \tau^{1/2}$

(1) $\beta = 0$ (no evaporation)

$f = \frac{6}{\pi^{1/2}} \tau^{1/2} - 3\tau$

(2) $\beta = 2$

(3) $\beta = 10$

(4) $\beta = 20$

(5) $\beta = 50$

(6) $\beta = 100$

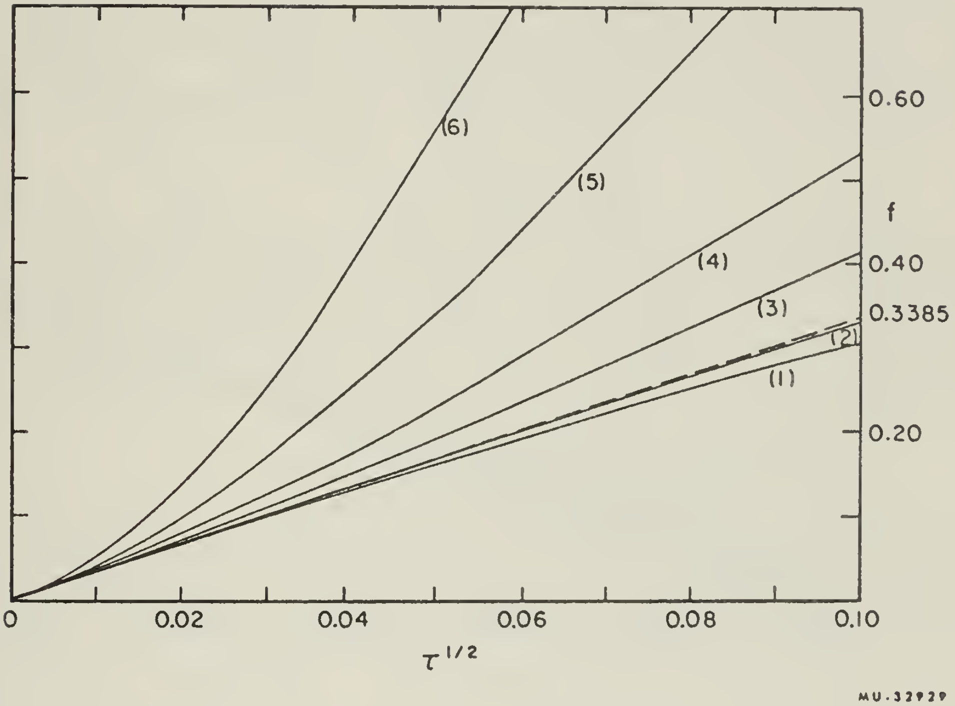

Fig. III. 1. Fractional release vs $\tau^{1/2}$ for various rates of evaporation.

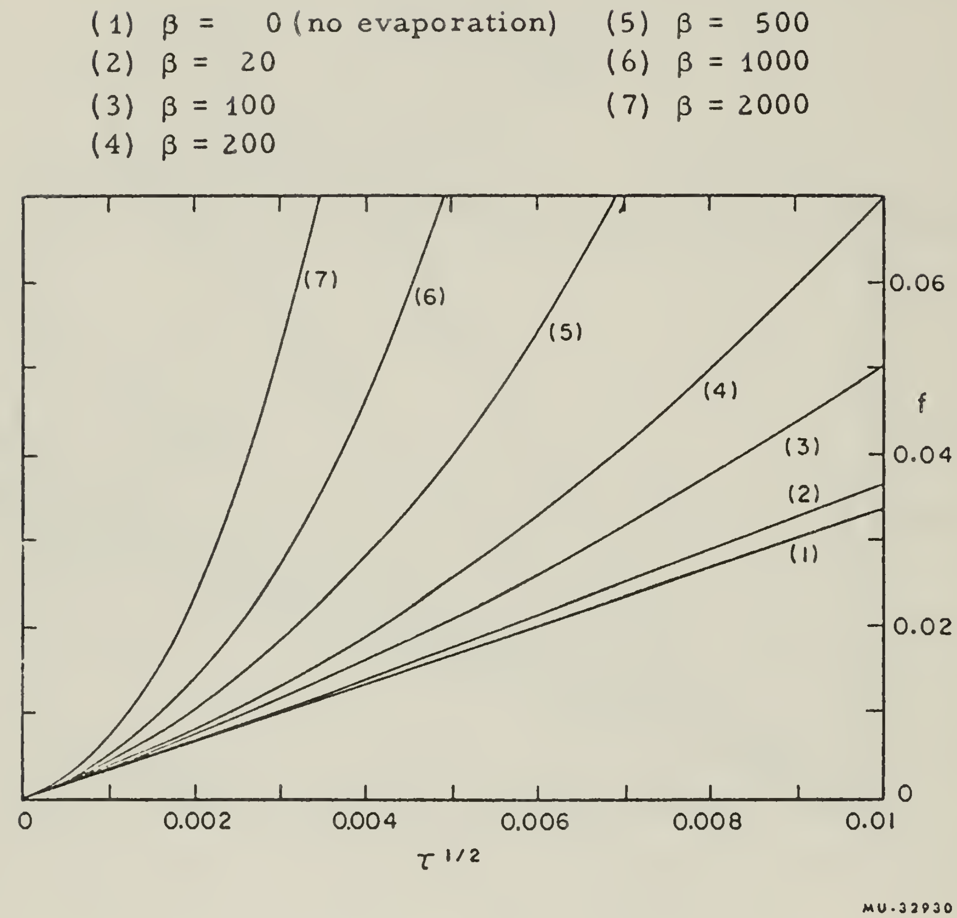

Fig. III. 2. Fractional release vs $\tau^{1/2}$ for various rates of evaporation.

IV. DISCUSSION

A. General Results

For all values of $\beta > 0$, the fractional release with time is increased over the corresponding value for f when $\beta = 0$. For any value of time (or τ), f will increase, for both the slab and sphere cases, as β increases. With smaller values of β, say $\beta < 20$, the curve of f vs $\tau^{1/2}$ very closely approximates a straight line for $\tau^{1/2} < 0.01$, which indicates that f is proportional (or very nearly so) to $\tau^{1/2}$. The same statement may be made for $\tau^{1/2} < 0.1$, provided $\beta < 2$.

B. Initial Release

This theory does not account for the large early release rate in postanneal experiments noted by several observers.[1, 6] In these cases, the slope of the f vs $t^{1/2}$ curve decreased with increasing time until a region of more or less constant slope was attained.

C. Spherical Case--Stationary Boundary

Figure III.1 illustrates the effect upon f of neglecting the second term of Eq. (III-20). For values of $\tau^{1/2} < 0.01$, the difference in values of f resulting from lack of consideration of the second term of Eq. (III-20) is negligible. For larger values of $\tau^{1/2}$, the fractional release predicted by Eq. (III-22) becomes increasingly greater than that predicted by Eq. (III-20), and differs by 0.03 (≈ 10%) at $\tau^{1/2} = 0.1$. Since both Eq. (III-20) and Eq. (III-22) appear to be plotted as straight lines, an error of 17% in the value of D results for the above value of τ from neglecting this term. It is noted that Eq. (III-22) closely represents the release curve resulting from boundary motion for which $\beta = 2$.

D. Spherical Case--Moving Boundary

For values of $\tau^{1/2} < 0.01$, Eq. (III-21) may be used in preference to Eq. (III-19) for all values of $\beta\tau$. If $\beta\tau$ (remember $\beta\tau$ independent of D and is bounded between 0 and 1) is approx$<$0.2, then the term $(\beta\tau)^3$ may also be neglected.

For large values of $\frac{1}{2}\beta\tau^{1/2}$, the fractional release is approximated by $3\beta\tau(1-\beta\tau)+(\beta\tau)^3$, which is a cubic equation in time (or τ). This may occur at short times for very rapid boundary motion (β), or for very long periods of time (τ). Neither of these cases, however, is useful in making a determination of D.

For small values of $\frac{1}{2}\beta\tau^{1/2}$, pertaining both to relatively short periods of time and small rates of boundary motion, the fractional release is directly proportional (or very nearly so) to $\tau^{1/2}$ and therefore to $\tau^{1/2}$. It should be possible, therefore, to develop a simple expression that may be used to determine D with greater accuracy than would the use of Eq. (III-22). For small $\frac{\beta\tau^{1/2}}{2}$, $\left(\frac{\beta\tau^{1/2}}{2} < 0.2\right)$; hence, Eq. (III-21) may be approximated by

$$f = \frac{3}{2}\beta\tau + \frac{6}{\pi^{1/2}}\tau^{1/2} = \frac{3}{2}\left(\frac{bt}{a}\right) + \frac{6}{\pi^{1/2}}\left(\frac{Dt}{a^2}\right)^{1/2}. \tag{IV-1}$$

With Eq. (IV-1), one can predict the release curve to be parabolic in shape when f is plotted vs time to the one-half power; the curvature depends upon b. The curve consists of a straight-line component and a parabolic component, which is the evaporation correction.

Figure IV.1 is the graphical presentation of Eq. (IV-1) for those values of f that do not differ by more than approximately 0.001 from the more accurate expression for f.

By assuming that b (the rate of boundary movement) has been determined, a corrected value of the fractional release may be obtained by subtracting the quantity $\frac{3}{2}\left(\frac{bt}{a}\right)$ from the actual fractional release. This corrected value of f may then be used with Eq. (III-22) to determine D.

E. Slab Case--Moving Boundary

For large values of $\frac{1}{2}\beta\tau^{1/2}$, the fractional release is approximated by $\beta\tau$--the percent of the body that has sublimed.

For small values of $\frac{\beta\tau^{1/2}}{2}$, $\left(\frac{\beta\tau^{1/2}}{2} < 0.2\right)$, a simplified expression for the fractional release may be developed in a manner similar to that for the spherical case. This is written as

$$f \approx \frac{3}{2}\,\beta\tau + \frac{6}{\pi^{1/2}}\,\tau^{1/2}$$

(1) β = 0 (no evaporation)
(2) β = 20
(3) β = 100
(4) β = 200
(5) β = 500
(6) β = 1000

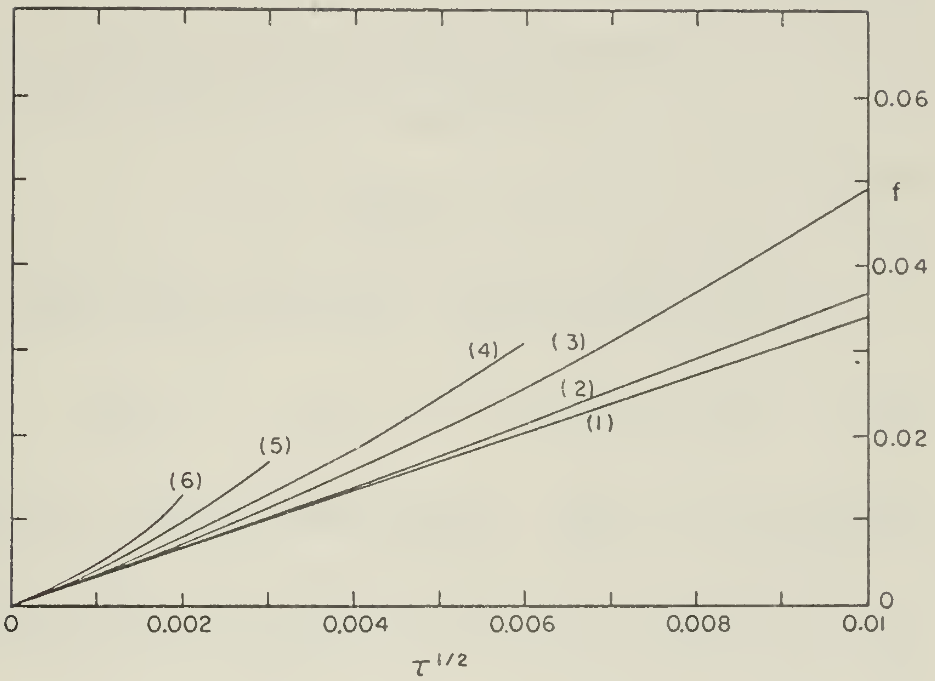

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Fig. IV. 1. Simplified expression for fractional release for the sphere.

$$f = \frac{1}{2}\beta\tau + \frac{2}{\pi^{1/2}}\tau^{1/2} = \frac{1}{2}\left(\frac{bt}{a}\right) + \frac{2}{\pi^{1/2}}\left(\frac{Dt}{a^2}\right)^{1/2} . \qquad \text{(IV-2)}$$

Hence, D may be determined in a manner similar to that for the spherical case. For small periods of time, the correction factor $\frac{1}{2}\beta\tau\left[\text{or } \frac{1}{2}\left(\frac{bt}{a}\right)\right]$ is negligible; thus a straight-line plot may be expected; and over longer time intervals the plot may be expected to show an increasing slope.

F. Some Numerical Considerations

Using the values of Shaked[1] for his sample # 108 at 2040°C, one obtains

$$D = 6.6 \times 10^{-12}\ \text{cm}^2/\text{sec},$$

$$t^{1/2} = 150\ (\text{sec})^{1/2} \qquad (t = 2.25 \times 10^4\ \text{sec}),$$

and $a = 0.25$ cm.

Therefore, $\tau = \frac{Dt}{a^2} = 2.38 \times 10^{-6} \quad (\tau^{1/2} = 1.54 \times 10^{-3})$.

The expected fractional release, with the use of Eq. (III-22), would be

$$f = \frac{6}{\pi^{1/2}}\tau^{1/2} = 5.2 \times 10^{-3} .$$

Shaked estimated that the value of b he encountered during the anneal of this sample was 0.3 μ/h. Because Shaked's sample was annealed in a Knudsen-type cell, this evaporation rate was considerably lower than would have occurred if the sample were completely exposed to vacuum.

Thus,

$$\beta = \frac{ba}{D} = 316,$$

and, if the value of f calculated above is substituted into Eq. (IV-1), one has

$$f = \frac{3}{2}\beta\tau + \frac{6}{\pi^{1/2}}\tau^{1/2} = \frac{3}{2}\left(\frac{bt}{a}\right) + \frac{6}{\pi^{1/2}}\left(\frac{Dt}{a^2}\right)^{1/2} = 5.2 \times 10^{-3},$$

with D representing a modified value of the diffusion constant

$$D = 4.1 \times 10^{-12}\ \mathrm{cm^2/sec},$$

which is 61% less than that calculated by neglecting evaporation.

If the sample had been completely exposed to vacuum at this temperature, the evaporation rate, b, estimated from thermodynamic data,[1] would be about 150 μ/h, from which

$$\beta = 158{,}000 .$$

For an anneal time of 2.25×10^4 sec and an actual D of 6.6×10^{-12} $\mathrm{cm^2/sec}$, it follows that

$$\frac{\beta\tau^{1/2}}{2} = 121 .$$

Using these data in Eq. (III-21), one predicts a fractional release of $f = 0.757$. Now, *if* the experiment had been performed in this way, and *if* the effects of evaporation were ignored, these values of f, t, and a used in the nonevaporation Eq. (III-22) would yield a value for D of

$$D = 13.9 \times 10^{-8}\ \mathrm{cm^2/sec},$$

which is approximately 21,000 times as large as the actual diffusion coefficient for this temperature.

These calculations illustrate the importance of either minimizing evaporation experimentally, or of taking it into account analytically whenever one obtains diffusion data at high temperatures.

V. CONCLUSIONS

An equation has been developed that relates the fractional release, f, of a tracer element in a geometrical body under conditions of evaporation of the body and diffusion of the tracer through the moving boundary of the body, with these conditions occurring simultaneously. This may be better expressed as the fractional release of the tracer element through a moving boundary.

For small values of the quantity β, the release curve is approximately a straight line whose slope is slightly greater than that for the stationary-boundary case. As β becomes larger in magnitude, the slope of the curve increases with increase in time and approaches a limiting value (see Fig. III.2) for the values of β and τ considered.

It can be seen that to completely ignore the evaporation of the body may lead to an incorrect value for the diffusion constant. The curve of f vs $(t)^{1/2}$ can appear to be a straight line when the boundary motion is not zero, but the slope of this line is not the same as that for the zero-boundary-motion line; hence, different values of D would be obtained unless a correction were applied to the moving-boundary case.

Simplified expressions have been developed that, for small values of the variable $\beta\tau^{1/2}/2$, may be used to make a more accurate determination of the diffusion constant, D. With these expressions one can predict a release curve whose slope, when f is plotted against the one-half power of time, will increase with time. The correction made to the fractional-release equation for the stationary-boundary case is independent of D, and by subtracting this correction from the actual release, one should obtain a line of constant slope.

It also should be possible to fit experimentally obtained fractional-release curves to the curves obtained in Sections II and III of this report, and thus to determine both the rate of boundary motion, b, and the diffusion constant, D.

Experimental verification of the simplified and the approximate relations for the fractional release remains to be demonstrated.

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APPENDIX

A. "Conventional" Analysis of the Slab Problem
B. "Conventional" Analysis of the Sphere Problem
C. Properties of the Error Functions and Related Functions
D. Solution of the Slab Problem for a Moving Boundary
E. Solution of the Sphere Problem for a Moving Boundary

APPENDIX

A. "Conventional" Analysis of the Slab Problem

Solutions to the heat-conduction equation for a slab $-a<x<a$, with a constant initial temperature T_0, and with $T=0$ at $x=\pm a$ are given as[7]

$$T(x,t)=\frac{4T_0}{\pi}\sum_{n=0}^{\infty}\frac{(-1)^n}{2n+1}\exp\left[-\frac{\kappa(2n+1)^2\pi^2 t}{4a^2}\right]\cos\frac{(2n+1)\pi x}{2a} \tag{A-1}$$

and

$$T(x,t)=T_0-T_0\sum_{n=0}^{\infty}(-1)^n\left\{\operatorname{erfc}\frac{(2n+1)a-x}{2(\kappa t)^{1/2}}+\operatorname{erfc}\frac{(2n+1)a+x}{2(\kappa t)^{1/2}}\right\}. \tag{A-2}$$

The average temperature in the slab is given as[7]

$$T_{av}=\frac{8T_0}{\pi^2}\sum_{n=0}^{\infty}\frac{1}{(2n+1)^2}\exp\left[-\frac{\kappa(2n+1)^2\pi^2 t}{4a^2}\right] \tag{A-3}$$

and

$$T_{av}=T_0-2T_0\left(\frac{\kappa t}{a^2}\right)^{1/2}\left\{\pi^{-1/2}+2\sum_{n=1}^{\infty}(-1)^n\operatorname{ierfc}\frac{na}{(\kappa t)^{1/2}}\right\}. \tag{A-4}$$

Using an analogy to the heat-conduction solution, it will be shown that the concentration of a tracer element $C(x,t)$ for any time t and any position x, where $-a<x<a$, the initial condition $C(x,0)=C_0$, where C_0 is a constant, is

$$C(x,t)=\frac{4C_0}{\pi}\sum_{n=0}^{\infty}\frac{(-1)^n}{2n+1}\exp\left[-\frac{(2n+1)^2\pi^2 Dt}{4a^2}\right]\cos\frac{(2n+1)\pi x}{2a} \tag{A-5}$$

and

$$C(x,t)=C_0-C_0\sum_{n=0}^{\infty}(-1)^n\left\{\operatorname{erfc}\frac{(2n+1)a-x}{2(Dt)^{1/2}}+\operatorname{erfc}\frac{(2n+1)a+x}{2(Dt)^{1/2}}\right\}. \tag{A-6}$$

Here, D is the diffusion coefficient for the particular element being studied. The corresponding fractional release, f, defined as the ratio of the decrease in average tracer concentration to the initial average concentration, is

$$f = \frac{C_0 - C_{av}(t)}{C_0} = 1 - \frac{8}{\pi^2} \sum_{n=0}^{\infty} \frac{1}{(2n+1)^2} \exp\left[-\frac{(2n+1)^2 \pi^2 D t}{4a^2}\right] \tag{A-7}$$

and

$$f = 2\left(\frac{Dt}{a^2}\right)^{1/2} \left\{\pi^{-1/2} + 2 \sum_{n=1}^{\infty} (-1)^n \, \mathrm{ierfc} \, \frac{na}{(Dt)^{1/2}}\right\} . \tag{A-8}$$

A.1. Tracer Concentration—Exponential Form

By using the method of separation of variables, it may be shown[8] that a solution for the diffusion equation

$$\frac{\partial C(x,t)}{\partial t} = D \frac{\partial^2 C(x,t)}{\partial x^2} , \tag{A-9}$$

with

$$C(x,0) = C_0 \tag{A-9a}$$

and

$$C(\pm a,t) = 0 , \tag{A-9b}$$

may be expressed as $C_n(x, t) = F_n(x)\, G_n(t)$, (A-10)

where

$$F_n(x) = A_n \cos k_n x + B_n \sin k_n x \tag{A-10a}$$

and

$$G_n(t) = \alpha \exp(-k_n^2 D t) . \tag{A-10b}$$

Applying the boundary conditions (A-9b), yields $B_n = 0$ and $k_n = \frac{\pi}{2a}(2n+1)$, where $n = 0, 1, 2, \cdots$. Applying the initial condition (A-9a) yields $\alpha = C_0$, so Eq. (A-10) becomes

$$\begin{aligned} C_n(x,t) &= C_o A_n \cos k_n x \exp(-k_n^2 Dt) \\ &= C_o A_n \cos\frac{(2n+1)\pi x}{2a} \exp\left[-\frac{(2n+1)^2\pi^2 Dt}{4a^2}\right]. \end{aligned} \qquad (A-11)$$

The coefficient A_n may be evaluated by setting $t = 0$ and using the property of a Fourier series[9] that

$$a_n = \frac{1}{\ell}\int_{-\ell}^{\ell} f(x) \cos\frac{n\pi x}{\ell}\, dx\ ; \qquad (A-12)$$

thus, $$A_n = \frac{1}{a}\int_{-a}^{a} f(x) \cos\frac{(2n+1)\pi x}{2a}\, dx\ , \qquad \text{where } f(x) = 1. \qquad (A-13)$$

This may be integrated directly to yield

$$A_n = \frac{4(-1)^n}{\pi(2n+1)}, \qquad n = 0, 1, 2 \cdots . \qquad (A-14)$$

Therefore, the substitution of Eq. (A-14) into Eq. (A-11) gives

$$C_n(x,t) = \frac{4C_o(-1)^n}{\pi(2n+1)} \exp\left[-\frac{(2n+1)^2\pi^2 Dt}{4a^2}\right] \cos\frac{(2n+1)\pi x}{2a} . \qquad (A-15)$$

Any sum of solutions is also a solution, so the final result is

$$C(x,t) = \frac{4C_o}{\pi}\sum_{n=0}^{\infty}\frac{(-1)^n}{2n+1} \exp\left[-\frac{(2n+1)^2\pi^2 Dt}{4a^2}\right] \cos\frac{(2n+1)\pi x}{2a} . \qquad (A-16)$$

For long periods of time, the tracer concentration should become zero as t → ∞. By noting that the exponent in each term approaches

$-\infty$ as $t \rightarrow \infty$, it is clear that the tracer concentration will indeed approach zero as a limit.

A.2. Fractional Release—Exponential Form

The fractional release, f, may be determined from

$$f = \frac{Q_0 - Q(t)}{Q_0}, \qquad \text{(A-17)}$$

where $Q(t)$ is the total number of tracer atoms per unit area contained in the solid at any time t, and $Q_0 = 2aC_0$ is the total number of tracer atoms per unit area contained in the solid at time $t = 0$:

$$f = \frac{2aC_0 - \int_{-a}^{a} C(x,t)\,dx}{2aC_0}$$

$$= 1 - \frac{1}{2aC_0}\,\frac{4C_0}{\pi}\sum_{n=0}^{\infty}\frac{(-1)^n}{2n+1}\exp\left[-\frac{(2n+1)^2\pi^2 Dt}{4a^2}\right]\int_{-a}^{a}\cos\frac{(2n+1)\pi x}{2a}\,dx \qquad \text{(A-18)}$$

$$= 1 - \frac{8}{\pi^2}\sum_{n=0}^{\infty}\frac{1}{(2n+1)^2}\exp\left[-\frac{(2n+1)^2\pi^2 Dt}{4a^2}\right].$$

For $t \rightarrow \infty$, the summation term approaches 0 as a limit; hence, the fractional release approaches 1 as a limit. For $t = 0$, Eq. (A-18) becomes

$$f = 1 - \frac{8}{\pi^2}\sum_{n=0}^{\infty}\frac{1}{(2n+1)^2}\,. \qquad \text{(A-19)}$$

The sum $\frac{1}{1^2} + \frac{1}{3^2} + \frac{1}{5^2} + \cdots = \sum_{n=0}^{\infty}\frac{1}{(2n+1)^2}$ is shown[9] to be equal to $\frac{\pi^2}{8}$, so $f = 1 - \frac{8}{\pi^2} \times \frac{\pi^2}{8} = 1 - 1 = 0$ at time $t = 0$, which is as expected.

Thus, it has been demonstrated how Eqs. (A-5) and (A-7) were obtained, and it has further been shown that the tracer concentration and the fractional release approach the proper limits for large periods of time, and at time t = 0.

It will now be shown, with the use of La Place transforms, that Eqs. (A-6) and (A-8) are the solutions of Eqs. (A-9) and (A-17), respectively.[7]

A.3. Tracer Concentration—Error-Function Form

Let
$$\frac{\partial C(x,t)}{\partial t} = D\,\frac{\partial^2 C(x,t)}{\partial x^2}, \qquad \text{(A-9)}$$

with
$$C(x,0) = C_0 \qquad \text{(A-9a)}$$

and
$$C(\pm a,t) = 0; \qquad \text{(A-9b)}$$

by symmetry,
$$\frac{\partial C(0,t)}{\partial x} = 0. \qquad \text{(A-20)}$$

Now the La Place transform of C(x, t) = $\bar{C}$(x, p);

$$\bar{C}(x,p) = \int_0^\infty e^{-pt}\,C(x,t)\,dt. \qquad \text{(A-21)}$$

Making the transformations of Eqs. (A-9), (A-9b), and (A-20), one obtained

$$p\bar{C}(x,p) - C_0 = D\,\frac{\partial^2 \bar{C}(x,p)}{\partial x^2}, \qquad \text{(A-22)}$$

with
$$\bar{C}(\pm a,p) = 0 \qquad \text{(A-22a)}$$

and
$$\frac{\partial \bar{C}(0,p)}{\partial x} = 0. \qquad \text{(A-22b)}$$

Defining $q^2 = p/D$ and by substituting in Eq. (A-22), one obtains

$$\frac{\partial^2 \bar{C}(x,p)}{\partial x^2} - q^2 \bar{C}(x,p) = -\frac{C_0}{D} . \qquad \text{(A-24)}$$

Solving Eq. (A-24) for $\bar{C}(x, p)$, one has

$$\bar{C}(x,p) = Ae^{qx} + Be^{-qx} + \frac{C_0}{p} . \qquad \text{(A-25)}$$

Upon applying Eq. (A-22a) and Eq. (A-22b) to Eq. (A-25), it follows that

$$\bar{C}(x,p) = -\frac{C_0(e^{qx}+e^{-qx})}{p\,(e^{qa}+e^{-qa})} + \frac{C_0}{p} . \qquad \text{(A-26)}$$

Multiplying the first term top and bottom by e^{-qa}, one sees that

$$\bar{C}(x,p) = -\frac{C_0}{p}\left[e^{q(x-a)}+e^{-q(x+a)}\right]\left[1+e^{-2qa}\right]^{-1} + \frac{C_0}{p} , \qquad \text{(A-27)}$$

and upon expanding $(1+e^{-2qa})^{-1}$ by the binomial theorem, one finds

$$\begin{aligned}\left[1+e^{-2qa}\right]^{-1} &= 1 - e^{-2qa} + (e^{-2qa})^2 - (e^{-2qa})^3 + \cdots \\ &= \sum_{n=0}^{\infty}(-1)^n e^{-2nqa} .\end{aligned} \qquad \text{(A-28)}$$

By substituting (A-28) into Eq. (A-27), it follows that

$$\begin{aligned}\bar{C}(x,p) &= -\frac{C_0}{p}\sum_{n=0}^{\infty}(-1)^n e^{-2nqa}\left[e^{q(x-a)} + e^{-q(x+a)}\right] + \frac{C_0}{p} \\ &= \frac{C_0}{p} - \frac{C_0}{p}\sum_{n=0}^{\infty}(-1)^n e^{-q[(2n+1)a-x]} - \frac{C_0}{p}\sum_{n=0}^{\infty}(-1)^n e^{-q[(2n+1)a+x]} .\end{aligned} \qquad \text{(A-29)}$$

Taking the inverse transforms, one obtains

$$C(x,t) = C_0 - C_0 \sum_{n=0}^{\infty} (-1)^n \left[\operatorname{erfc} \frac{(2n+1)a-x}{2(Dt)^{1/2}} + \operatorname{erfc} \frac{(2n+1)a+x}{2(Dt)^{1/2}} \right]. \qquad \text{(A-30)}$$

For long periods of time, the tracer concentration should become zero as $t \rightarrow \infty$. If t is allowed to approach infinity in Eq. (A-30), the $\operatorname{erfc} \frac{k}{t} \rightarrow 1.0$, and Eq. (A-30) becomes

$$\begin{aligned} \lim_{t \to \infty} C(x,t) &= C_0 - C_0 \sum_{n=0}^{\infty} (-1)^n (2) \\ &= C_0 - C_0 (2 - 2 + 2 - 2 + \cdots), \end{aligned} \qquad \text{(A-31)}$$

which appears to be nonconvergent and equals C_0 or $-C_0$, depending upon whether the last term of the expansion is negative or positive. This is a periodic function, however; and if the function $f(x)$ is defined as

$$f(x) = 2 \quad \text{if} \quad 0 \leqslant x \leqslant \pi, \qquad \text{(A-32a)}$$

and

$$f(x) = 0 \quad \text{if} \quad -\pi \leqslant x \leqslant 0, \qquad \text{(A-32b)}$$

then the coefficients of the Fourier series for $f(x)$ are

$$a_0 = \frac{1}{\pi}\int_{-\pi}^{0} 0\,dx + \frac{1}{\pi}\int_0^{\pi} 2\,dx = 2, \qquad \text{(A-33a)}$$

$$a_n = \frac{1}{\pi}\int_0^{\pi} 2\cos nx\,dx = \frac{2}{\pi n} \sin nx \Big]_0^{\pi} = 0, \qquad \text{(A-33b)}$$

and

$$b_n = \frac{1}{\pi}\int_0^{\pi} 2\sin nx\,dx = \frac{-2}{n\pi}\cos nx \Big]_0^{\pi} = \frac{2}{n\pi}(1-\cos n\pi), \qquad \text{(A-33c)}$$

and the Fourier series for $f(x)$ becomes

$$\begin{aligned} f(x) &= \frac{1}{2}a_0 + \sum_{n=1}^{\infty} (a_n \cos nx + b_n \sin nx) \\ &= 1 + \frac{4}{\pi}\left(\frac{\sin x}{1} + \frac{\sin 3x}{3} + \frac{\sin 5x}{5} + \cdots\right) = \end{aligned}$$

$$= 1 + \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{1}{2n+1} \sin(2n+1)x \, . \tag{A-34}$$

On page 180 of Sokolonikoff and Redheffer,[9] it may be seen that f(x) is well-defined on the closed interval $-\pi \leqslant x \leqslant \pi$ except for the simple discontinuity at $x = 0$, has a finite number of maxima and minima, and is defined for other values of x by the periodicity condition $f(x+2\pi) = f(x)$; therefore, the Dirichlet conditions hold for f(x), and the Fourier series for f(x) converges to

$$f(x) = \frac{1}{2}\left[f(x^+) + f(x^-)\right] \tag{A-35}$$

for every value of x.

In particular, at $x = 0$,

$$f(0) = \frac{1}{2}\left[f(0^+) + f(0^-)\right] = \frac{1}{2}(2+0) = 1 \, . \tag{A-36}$$

Because the coefficient of the second term in Eq. (A-31) is shown to converge to the value 1, the tracer concentration will, in fact, approach zero as a limit as $t \to \infty$.

A.4. Fractional Release—Error-Function Form

Calculating the fractional release from Eq. (A-17), one obtains

$$f = \frac{2aC_0 - \int_{-a}^{a} C(x,t)\,dx}{2aC_0}$$

$$= 1 - \frac{1}{2aC_0}\int_{-a}^{a}\left\{C_0 - C_0\left[\sum_{n=0}^{\infty}(-1)^n \operatorname{erfc}\frac{(2n+1)a-x}{2(Dt)^{1/2}} + \sum_{n=0}^{\infty}(-1)^n \operatorname{erfc}\frac{(2n+1)a+x}{2(Dt)^{1/2}}\right]\right\}dx \tag{A-37}$$

$$= \frac{1}{2a}\int_{-a}^{a}\left[\sum_{n=0}^{\infty}(-1)^n \operatorname{erfc}\frac{(2n+1)a-x}{2(Dt)^{1/2}} + \sum_{n=0}^{\infty}(-1)^n \operatorname{erfc}\frac{(2n+1)a+x}{2(Dt)^{1/2}}\right]dx \, ,$$

which, with the use of Eq. (C-11), becomes

$$f = \frac{2(Dt)^{1/2}}{2a}\left\{\sum_{n=0}^{\infty}(-1)^n\left[\operatorname{ierfc}\frac{(2n+1)a-a}{2(Dt)^{1/2}} - \operatorname{ierfc}\frac{(2n+1)a+a}{2(Dt)^{1/2}}\right]\right.$$

$$\left. - \sum_{n=0}^{\infty}(-1)^n\left[\operatorname{ierfc}\frac{(2n+1)a+a}{2(Dt)^{1/2}} - \operatorname{ierfc}\frac{(2n+1)a-a}{2(Dt)^{1/2}}\right]\right\}$$

$$= 2\left(\frac{Dt}{a^2}\right)^{1/2}\left\{\sum_{n=0}^{\infty}(-1)^n\left[\operatorname{ierfc}\frac{na}{(Dt)^{1/2}} - \operatorname{ierfc}\frac{(n+1)a}{(Dt)^{1/2}}\right]\right\} \qquad \text{(A-38)}$$

$$= 2\left(\frac{Dt}{a^2}\right)^{1/2}\left[\operatorname{ierfc} 0 + \sum_{n=1}^{\infty}(-1)^n \operatorname{ierfc}\frac{na}{(Dt)^{1/2}} - \sum_{n=0}^{\infty}(-1)^n \operatorname{ierfc}\frac{(n+1)a}{(Dt)^{1/2}}\right].$$

By letting $n + 1 = m$, the last two terms may be combined, and by noting, from Eq. (C-7), that ierfc $0 = \pi^{-1/2}$, one finds Eq. (A-38) to be

$$f = 2\left(\frac{Dt}{a^2}\right)^{1/2}\left[\pi^{-1/2} + 2\sum_{n=1}^{\infty}(-1)^n \operatorname{ierfc}\frac{na}{(Dt)^{1/2}}\right]. \qquad \text{(A-39)}$$

For $t \rightarrow 0$, the terms in Eq. (A-39) involving ierfc $k/t^{1/2}$ become zero; thus, only the first term $\frac{2}{\pi^{1/2}}\left(\frac{Dt}{a^2}\right)^{1/2}$ remains. For $t = 0$, this term and also the fractional release are zero.

For large t, as $t \rightarrow \infty$, the terms involving the ierfc $na/(Dt)^{1/2} \rightarrow$ ierfc 0, where ierfc $0 = \pi^{-1/2}$; with these substitutions Eq. (A-39) becomes

$$\lim_{t\to\infty} f = \frac{2}{\pi^{1/2}}\left(\frac{Dt}{a^2}\right)^{1/2}\left[1 + 2\sum_{n=1}^{\infty}(-1)^n\right]. \qquad \text{(A-40)}$$

By using the same analysis as that for the tracer concentration, it can be shown that the summation term converges to -1; thus Eq. (A-40) is

$$\lim_{t\to\infty} f = \frac{2}{\pi^{1/2}}\left(\frac{Dt}{a^2}\right)^{1/2}[1-1] = \infty \cdot 0,$$

which is indeterminate; therefore, it is necessary to refer to Eq. (A-37) to resolve the indeterminateness. Hence,

$$\lim_{t\to\infty} f = \frac{1}{2a}\int_{-a}^{a} \lim_{t\to\infty}\Big[\sum_{n=0}^{\infty}(-1)^n \operatorname{erfc}\frac{(2n+1)a-x}{2(Dt)^{1/2}} + \sum_{n=0}^{\infty}(-1)^n \operatorname{erfc}\frac{(2n+1)a+x}{2(Dt)^{1/2}}\Big]dx$$

$$= \frac{1}{2a}\int_{-a}^{a}\Big[\sum_{n=0}^{\infty}(-1)^n(1) + \sum_{n=0}^{\infty}(-1)^n(1)\Big]dx \qquad \text{(A-41)}$$

$$= \frac{1}{2a}\int_{-a}^{a} 2\sum_{n=0}^{\infty}(-1)^n dx = 2\sum_{n=0}^{\infty}(-1)^n\left(\frac{1}{2a}\right)\int_{-a}^{a} dx$$

$$= 2\sum_{n=0}^{\infty}(-1)^n .$$

This previously was shown to be 1, so

$$\lim_{t\to\infty} f = 1 . \qquad \text{(A-42)}$$

It has now been shown how Eqs. (A-6) and (A-8) were obtained, and it has further been demonstrated that the tracer concentration and the fractional release approach the proper limits for large periods of time, and at time t = 0.

A.5. Correlation Between the Two Forms for Fractional Release

Using the method of Booth,[6] one can show that Eqs. (A-7) and (A-8) are identical for values of $\frac{\pi^2 Dt}{a^2} < 1$. Here,

$$f = 1 - \frac{8}{\pi^2}\sum_{n=0}^{\infty}\frac{1}{(2n+1)^2}\exp\left[-\frac{(2n+1)^2\pi^2 Dt}{4a^2}\right] \qquad \text{(A-7)}$$

for $\frac{\pi^2 Dt}{a^2} < 1$. Equation (A-8) becomes

$$f = \frac{2}{\pi^{1/2}}\left(\frac{Dt}{a^2}\right)^{1/2} . \qquad \text{(A-8a)}$$

Rewriting Eq. (A-7), one has

$$f = 1 - \frac{8}{\pi^2}\left[\sum_{n=1}^{\infty}\frac{1}{n^2}e^{-\frac{n^2\pi^2 Dt}{4a^2}} - \sum_{m=1}^{\infty}\frac{1}{(2m)^2}e^{-\frac{(2m)^2\pi^2 Dt}{4a^2}}\right]. \qquad \text{(A-43)}$$

The sum $\sum_{m=-\infty}^{\infty} e^{-m^2x} = 1 + 2\sum_{m=1}^{\infty} e^{-m^2x}$ (A-44)

is, for small x, essentially $\int_{-\infty}^{\infty} e^{-xu^2}\,du$. Thus,

$$\int_{-\infty}^{\infty} e^{-xu^2}\,du = (\pi/x)^{1/2}, \qquad \text{(A-45)}$$

where x for this case is $\frac{K\pi^2 Dt}{4a^2}$, K is 1 or 4, such that

$$1 + 2\sum_{m=1}^{\infty} e^{-m^2x} = (\pi/x)^{1/2}. \qquad \text{(A-46)}$$

Now, if both sides of Eq. (A-46) are integrated over the limits 0 to x, the result is

$$x + 2\sum_{m=1}^{\infty}\frac{1}{m^2}\left(1 - e^{-m^2x}\right) = 2(\pi x)^{1/2}, \qquad \text{(A-47)}$$

which may be arranged

$$-\sum_{m=1}^{\infty}\frac{1}{m^2}e^{-m^2x} = (\pi x)^{1/2} - \frac{x}{2} - \sum_{m=1}^{\infty}\frac{1}{m^2}. \qquad \text{(A-48)}$$

Upon substituting Eq. (A-48) into Eq. (A-43), one finds,

$$f = 1 + \frac{8}{\pi^2}\left[(\pi x_1)^{1/2} - \frac{x_1}{2} - \sum_{n=1}^{\infty}\frac{1}{n^2}\right]$$
$$- \frac{8}{\pi^2}\left\{\frac{1}{4}\left[(\pi x_2)^{1/2} - \frac{x_2}{2} - \sum_{m=1}^{\infty}\frac{1}{m^2}\right]\right\} =$$

$$= 1 + \frac{8}{\pi^2}\left[\left(\frac{\pi^3 Dt}{4a^2}\right)^{1/2} - \frac{\pi^2 Dt}{8a^2} - \sum_{n=1}^{\infty}\frac{1}{n^2}\right]$$

$$- \frac{8}{\pi^2}\left\{\frac{1}{4}\left[\left(\frac{4\pi^3 Dt}{4a^2}\right)^{1/2} - \frac{4\pi^2 Dt}{8a^2} - \sum_{m=1}^{\infty}\frac{1}{m^2}\right]\right\}. \qquad \text{(A-49)}$$

$$= 1 + \frac{2}{\pi^{1/2}}\left(\frac{Dt}{a^2}\right)^{1/2} - \frac{6}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2}.$$

The $\sum_{n=1}^{\infty}\frac{1}{n^2}$ is shown[9] as equal to $\frac{\pi^2}{6}$; hence,

$$f = \frac{2}{\pi^{1/2}}\left(\frac{Dt}{a^2}\right)^{1/2}. \qquad \text{(A-50)}$$

For values of $\frac{\pi^2 Dt}{a^2} < 1$, Eq. (A-8) reduces to Eq. (A-50); thus, for these values of $\frac{\pi^2 Dt}{a^2}$, Eqs. (A-7) and (A-8) are equivalent.

Solutions of the form of Eq. (A-7) converge slowly for small values of Dt/a^2, but solutions of the form (A-8) are rapidly convergent for the same small values.[7] This statement also applies to the equations for the tracer concentration, i.e., to Eqs. (A-5) and (A-6).

B. "Conventional" Analysis of the Sphere Problem

Solutions to the heat-conduction equation for a sphere, $0 < r < a$, with a constant initial temperature T_0, with $T = 0$ at $r = a$, and with T finite at $r = 0$, are given as[7]

$$T(r,t) = -\frac{2aT_0}{\pi r}\sum_{n=1}^{\infty}\frac{(-1)^n}{n}\exp\left(-\frac{n^2\pi^2 kt}{a^2}\right)\sin\frac{n\pi r}{a}\ , \qquad \text{(B-1)}$$

$$T(0,t) = -2T_0\sum_{n=1}^{\infty}(-1)^n\exp\left(-\frac{n^2\pi^2 kt}{a^2}\right)\ ; \qquad \text{(B-1a)}$$

and

$$T(r,t) = T_0 - \frac{aT_0}{r}\sum_{n=0}^{\infty}\left[\text{erfc}\frac{(2n+1)a-r}{2(kt)^{1/2}} - \text{erfc}\frac{(2n+1)a+r}{2(kt)^{1/2}}\right]\ , \qquad \text{(B-2)}$$

$$T(0,t) = T_0 - \frac{aT_0}{(\pi kt)^{1/2}}\sum_{n=0}^{\infty}\exp\left[-\frac{(2n+1)^2a^2}{4kt}\right]\ . \qquad \text{(B-2a)}$$

[See note following Eq. (B-6a).]

The average temperature in the sphere is given as[7]

$$T_{av} = \frac{6T_0}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2}\exp\left(-\frac{kn^2\pi^2 t}{a^2}\right) \qquad \text{(B-3)}$$

and

$$T_{av} = T_0 - 6T_0\left(\frac{kt}{a^2}\right)^{1/2}\left[\pi^{-1/2} + 2\sum_{n=1}^{\infty}\text{ierfc}\frac{na}{(kt)^{1/2}}\right] + 3T_0\left(\frac{kt}{a^2}\right)\ . \qquad \text{(B-4)}$$

Using an analogy to the heat-conduction solution, one can show that the concentration of a tracer element $C(r, t)$ for any time t and any position r, where $0 < r < a$ and the initial condition $C(r, 0) = C_0$, with C_0 a constant and with $C(0, t)$ finite, is

$$C(r,t) = -\frac{2aC_0}{\pi r}\sum_{n=1}^{\infty}\frac{(-1)^n}{n}\exp\left(-\frac{n^2\pi^2 Dt}{a^2}\right)\sin\frac{n\pi r}{a}, \tag{B-5}$$

$$C(0,t) = -2C_0\sum_{n=1}^{\infty}(-1)^n\exp\left(-\frac{n^2\pi^2 Dt}{a^2}\right); \tag{B-5a}$$

and

$$C(r,t) = C_0 - \frac{aC_0}{r}\sum_{n=0}^{\infty}\left[\operatorname{erfc}\frac{(2n+1)a-r}{2(Dt)^{1/2}} - \operatorname{erfc}\frac{(2n+1)a+r}{2(Dt)^{1/2}}\right], \tag{B-6}$$

$$C(0,t) = C_0 - \frac{2aC_0}{(\pi Dt)^{1/2}}\sum_{n=0}^{\infty}\exp\left[-\frac{(2n+1)^2a^2}{4Dt}\right]. \tag{B-6a}$$

[It will be noted that Eq. (B-6a) differs from (B-2a)--other than in the change of notation--by a factor of two in the summation term. It will subsequently be shown that Eq. (B-6a) is the proper expression for the tracer concentration at the center of the sphere.]

The corresponding equations for the fractional release of the tracer element are

$$f = 1 - \frac{6}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2}\exp\left(-\frac{n^2\pi^2 Dt}{a^2}\right) \tag{B-7}$$

and

$$f = 6\left(\frac{Dt}{a^2}\right)^{1/2}\left[\pi^{-1/2} + 2\sum_{n=1}^{\infty}\operatorname{ierfc}\frac{na}{(Dt)^{1/2}}\right] - 3\left(\frac{Dt}{a^2}\right). \tag{B-8}$$

B.1. Tracer Concentration—Exponential Form

The radial-diffusion equation

$$\frac{\partial C(r,t)}{\partial t} = D\left[\frac{\partial^2 C(r,t)}{\partial r^2} + \frac{2}{r}\frac{\partial C(r,t)}{\partial r}\right] \tag{B-9}$$

may be reduced to the linera-diffusion equation (A-9) by making the substitution $u(r, t) = rC(r, t)$

$$\frac{\partial u(r,t)}{\partial t} = D \frac{\partial^2 u(r,t)}{\partial r^2} , \tag{B-10}$$

with the following boundary and initial conditions

$$u(r, 0) = rC_0 , \tag{B-10a}$$

$$u(a, t) = 0 , \tag{B-10b}$$

and

$$u(0, t) = 0 . \tag{B-10c}$$

A solution for Eq. (B-10) may be obtained by using the method of separation of variables[8]

$$U_n(r, t) = F_n(r)\, G_n(t) , \tag{B-11}$$

where

$$F_n(r) = A_n \cos k_n r + B_n \sin k_n r , \tag{B-11a}$$

and

$$G_n(t) = \alpha\, e^{-k_n^2 Dt} . \tag{B-11b}$$

Applying the boundary condition (B-10c) yields $A_n = 0$. The boundary condition (B-10b) gives $k_n = \frac{n\pi}{a}$, whereas Eq. (B-10a) gives $\alpha = C_0$, $(n = 1, 2, 3 \cdots)$, and Eq. (B-11) becomes

$$\begin{aligned} U_n(r,t) &= C_0 B_n \sin k_n r \exp(-k_n^2 Dt) \\ &= C_0 B_n \sin \frac{n\pi r}{a} \exp\left(-\frac{n^2\pi^2 Dt}{a^2}\right) . \end{aligned} \tag{B-12}$$

The coefficient B_n may be evaluated by setting $t = 0$ and by using the property of a Fourier series that[9]

$$b_n = \frac{1}{l}\int_{-l}^{l} f(x) \sin \frac{n\pi x}{l}\, dx ; \tag{B-13}$$

Thus,

$$B_n = \frac{1}{a}\int_{-a}^{a} f(r) \sin \frac{n\pi r}{a}\, dr \,, \qquad \text{where} \qquad f(r) = r \,. \qquad \text{(B-14)}$$

This may be integrated by parts to give

$$B_n = -\frac{2a}{\pi n}(-1)^n \quad , \qquad (n = 1, 2, 3, \cdots). \qquad \text{(B-15)}$$

The substitution of Eq. (B-15) into Eq. (B-12) results in

$$U_n(r,t) = -\frac{2aC_0(-1)^n}{\pi n} \exp\left[-\frac{n^2\pi^2 Dt}{a^2}\right] \sin \frac{n\pi r}{a} \,. \qquad \text{(B-16)}$$

Any sum of solutions is also a solution; so the final result, upon using $C(r, t) = \frac{1}{r} u(r, t)$, is

$$C(r,t) = -\frac{2aC_0}{\pi r} \sum_{n=1}^{\infty} \frac{(-1)^n}{n} \exp\left[-\frac{n^2\pi^2 Dt}{a^2}\right] \sin \frac{n\pi r}{a} \qquad \text{(B-17)}$$

and

$$C(0,t) = \lim_{r\to 0} C(r,t) = -2C_0 \sum_{n=1}^{\infty} (-1)^n \exp\left[-\frac{n^2\pi^2 Dt}{a^2}\right] , \qquad \text{(B-17a)}$$

where the relation

$$\lim_{x\to 0} \frac{\sin x}{x} = 1$$

has been used.

For long periods of time, the tracer concentration should become zero as t → ∞. By noting that the exponent in each term in both Eqs. (B-17) and (B-17a) approaches $-\infty$ as t → ∞, it is clear that the tracer concentration will indeed approach zero as a limit.

B.2. Fractional Release — Exponential Form

The fractional release may be determined from

$$f = \frac{Q_0 - Q(t)}{Q_0} , \tag{A-17}$$

where $Q(t)$ is the total number of tracer atoms contained in the solid at any time t, and $Q_0 = \frac{4}{3}\pi a^3 C_0$ is the total number of tracer atoms contained in the solid at time $t = 0$. Thus,

$$f = \frac{4/3\,\pi a^3 C_0 - \int_0^a 4\pi r^2 C(r,t)\,dr}{4/3\,\pi a^3 C_0}$$

$$= 1 - \frac{3}{a^3 C_0}\left(-\frac{2aC_0}{\pi}\right)\sum_{n=1}^{\infty}\frac{(-1)^n}{n}\exp\left(-\frac{n^2\pi^2 Dt}{a^2}\right)\int_0^a r\sin\frac{n\pi r}{a}\,dr \tag{B-18}$$

$$= 1 - \frac{6}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2}\exp\left(-\frac{n^2\pi^2 Dt}{a^2}\right).$$

For $t \to \infty$, the summation term approaches zero as a limit; hence, the fractional release approaches 1 as a limit. For $t = 0$, Eq. (B-18) becomes

$$f = 1 - \frac{6}{\pi^2}\sum_{n=1}^{\infty}\frac{1}{n^2} . \tag{B-19}$$

The sum $\frac{1}{1^2} + \frac{1}{2^2} + \frac{1}{3^2} + \cdots = \sum_{n=1}^{\infty}\frac{1}{n^2}$ is shown[9] to be equal to $\frac{\pi^2}{6}$; so, $f = 1 - \frac{6}{\pi^2} \times \frac{\pi^2}{6} = 1 - 1 = 0$ at time $t = 0$, which is as expected.

Thus, it has been demonstrated how Eq. (B-5) and (B-7) were obtained. It has further been shown that the tracer concentration and the fractional release approach the proper limits for long periods of time and at time $t = 0$.

It will now be shown, by using La Place transforms,[7] that Eqs. (B-6) and (B-8) are the solutions of Eqs. (B-9) and (A-17), respectively.

B.3. Tracer Concentration—Error-Function Form

We have

$$\frac{\partial C(r,t)}{\partial t} = D\left[\frac{\partial^2 C(r,t)}{\partial r^2} + \frac{2}{r}\frac{\partial C(r,t)}{\partial r}\right], \tag{B-9}$$

with $$C(a, t) = 0 \quad , \tag{B-9a}$$

$$C(r, 0) = C_0 , \tag{B-9b}$$

and $$\frac{\partial C(0,t)}{\partial r} = 0 , \quad \text{by symmetry .} \tag{B-20}$$

The La Place transform of $C(r, t) = \bar{C}(r, p)$ is

$$\bar{C}(r,p) = \int_0^\infty e^{-pt} C(r,t)\, dt \ . \tag{B-21}$$

Making the transformations of Eqs. (B-9), (B-9a), and (B-20), one obtains

$$p\bar{C}(r,p) - C_0 = D\left[\frac{\partial^2 C(r,p)}{\partial r^2} + \frac{2}{r}\frac{\partial C(r,p)}{\partial r}\right], \tag{B-22}$$

where $$\bar{C}(a, p) = 0 , \tag{B-22a}$$

and $$\frac{\partial \bar{C}(0,p)}{\partial r} = 0 \ . \tag{B-22b}$$

Defining

$$q^2 = P/D \tag{B-23}$$

and substituting Eq. (B-23) in Eq. (B-22), one has

$$\frac{\partial^2 \bar{C}(r,p)}{\partial r^2} + \frac{2}{r}\frac{\partial \bar{C}(r,p)}{\partial r} - q^2 \bar{C}(r,p) = -\frac{C_0}{D} \ . \tag{B-24}$$

Solving Eq. (B-24) for $\bar{C}(r, p)$, one obtains

$$\bar{C}(r,p) = \frac{A}{r} e^{qr} + \frac{B}{r} e^{-qr} + \frac{C_0}{p} \ . \tag{B-25}$$

Upon applying Eqs. (B-22a) and (B-22b) to Eq. (B-25), it follows that

$$\bar{C}(r,p) = -\frac{C_0 a\,[e^{-qr} - e^{qr}]}{rp\,[e^{-qa} - e^{qa}]} + \frac{C_0}{p}. \qquad \text{(B-26)}$$

Then, multiplying the first term of Eq. (B-26) top and bottom by e^{-qa}, one finds

$$\bar{C}(r,p) = -\frac{C_0 a}{rp}\left[e^{-q(a-r)} - e^{-q(a+r)}\right]\left[1 - e^{-2qa}\right]^{-1} + \frac{C_0}{p}, \qquad \text{(B-27)}$$

and expanding $[1 - e^{-2qa}]^{-1}$ by the binomial theorem, one gets

$$\begin{aligned}\left[1 - e^{-2qa}\right]^{-1} &= 1 + e^{-2qa} + \left(e^{-2qa}\right)^2 + \left(e^{-2qa}\right)^3 + \cdots \qquad \text{(B-28)}\\ &= \sum_{n=0}^{\infty} e^{-2nqa}.\end{aligned}$$

Substituting Eq. (B-28) into Eq. (B-27), one sees that

$$\bar{C}(r,p) = \frac{C_0}{p} - \frac{C_0 a}{rp}\sum_{n=0}^{\infty}\left\{e^{-q[(2n+1)a-r]} - e^{-q[(2n+1)a+r]}\right\}. \qquad \text{(B-29)}$$

Upon taking the inverse transform, one finds

$$C(r,t) = C_0 - \frac{aC_0}{r}\sum_{n=0}^{\infty}\left[\mathrm{erfc}\,\frac{(2n+1)a-r}{2(Dt)^{1/2}} - \mathrm{erfc}\,\frac{(2n+1)a+r}{2(Dt)^{1/2}}\right] \qquad \text{(B-30)}$$

and

$$C(0,t) = \lim_{r\to 0} C(r,t) = C_0 - \frac{0}{0}, \qquad \text{(B-30a)}$$

which is indeterminate. Applying L'Hospital's rule[10] to the second term to eliminate the indeterminateness, one sees that

$$\lim_{x\to a}\frac{f(x)}{g(x)} = \lim_{x\to a}\frac{f'(x)}{g'(x)} = \cdots .$$

Now,

$$C(0,t) = C_0 - \lim_{r\to 0} \frac{aC_0}{r} \sum_{n=0}^{\infty} \left[\operatorname{erfc}\frac{(2n+1)a-r}{2(Dt)^{1/2}} - \operatorname{erfc}\frac{(2n+1)a+r}{2(Dt)^{1/2}} \right]$$

$$= C_0 - \lim_{r\to 0} \frac{aC_0}{1} \sum_{n=0}^{\infty} \left(\left[\frac{2}{\pi^{1/2}}\right]\left[\frac{1}{2(Dt)^{1/2}}\right] \exp\left\{-\left[\frac{(2n+1)a-r}{2(Dt)^{1/2}}\right]^2\right\} - \left[\frac{2}{\pi^{1/2}}\right]\left[\frac{-1}{2(Dt)^{1/2}}\right] \exp\left\{-\left[\frac{(2n+1)a+r}{2(Dt)^{1/2}}\right]^2\right\} \right) \qquad \text{(B-30b)}$$

$$= C_0 - \frac{aC_0}{(\pi Dt)^{1/2}} \lim_{r\to 0} \sum_{n=0}^{\infty} \left(\exp\left\{-\left[\frac{(2n+1)a-r}{2(Dt)^{1/2}}\right]^2\right\} + \exp\left\{-\left[\frac{(2n+1)a+r}{2(Dt)^{1/2}}\right]^2\right\} \right)$$

$$= C_0 - \frac{2aC_0}{(\pi Dt)^{1/2}} \sum_{n=0}^{\infty} \exp\left[-\frac{(2n+1)^2 a^2}{4Dt}\right].$$

As an additional check on Eq. (B-30b), it can be shown that the tracer concentration approaches zero as a limit as t → ∞.

The sum

$$\sum_{n=-\infty}^{\infty} e^{-n^2 x} = 1 + 2\sum_{n=1}^{\infty} e^{-n^2 x} \qquad \text{(A-44)}$$

is, for small x, essentially[6] $\int_{-\infty}^{\infty} e^{-xu^2}\,du$,

where $$\int_{-\infty}^{\infty} e^{-xu^2}\,du = \left(\frac{\pi}{x}\right)^{1/2}. \qquad \text{(A-45)}$$

Equation (B-30b) may be written as

$$C(0,t) = C_0 - \frac{2aC_0}{(\pi Dt)^{1/2}} \left\{ \sum_{n=1}^{\infty} \exp\left(-\frac{n^2 a^2}{4Dt}\right) - \sum_{n=1}^{\infty} \exp\left[-\frac{(2n)^2 a^2}{4Dt}\right] \right\}. \qquad \text{(B-31)}$$

Combining Eqs. (A-44) and (A-45), one finds that

$$\sum_{n=1}^{\infty} e^{-n^2 x} = \frac{1}{2}\left(\frac{\pi}{x}\right)^{1/2} - \frac{1}{2}\,; \qquad \text{(B-32)}$$

and by substituting Eq. (B-32) into Eq. (B-31), one obtains

$$\lim_{t\to\infty} C(0,t) = C_0 - \lim_{t\to\infty} \frac{2aC_0}{(\pi Dt)^{1/2}} \left[\frac{1}{2}\left(\frac{4\pi Dt}{a^2}\right)^{1/2} - \frac{1}{2}\left(\frac{\pi Dt}{a^2}\right)^{1/2}\right]$$

$$= C_0 - \lim_{t\to\infty} \frac{2aC_0}{2a(\pi Dt)^{1/2}} \left[2(\pi Dt)^{1/2} - (\pi Dt)^{1/2}\right] \qquad \text{(B-33)}$$

$$= C_0 - C_0 = 0 \, .$$

B.4. Fractional-Release — Error-Function Form

Calculating the fractional release from Eq. (A-17), one has

$$f = 1 - \frac{3}{a^3 C_0}\int_0^a r^2 C(r,t)\,dr$$

$$= 1 - \frac{3C_0}{a^3 C_0}\int_0^a r^2 \left\{1 - \frac{a}{r}\sum_{n=0}^{\infty}\left[\operatorname{erfc}\frac{(2n+1)a-r}{2(Dt)^{1/2}} - \operatorname{erfc}\frac{(2n+1)a+r}{2(Dt)^{1/2}}\right]\right\}dr \qquad \text{(B-34)}$$

$$= \frac{3}{a^2}\int_0^a r\sum_{n=0}^{\infty}\left[\operatorname{erfc}\frac{(2n+1)a-r}{2(Dt)^{1/2}} - \operatorname{erfc}\frac{(2n+1)a+r}{2(Dt)^{1/2}}\right]dr \, .$$

Now, Eq. (B-34) may be integrated by parts, by using Eq. (C-11) and by letting u = r and

$$dv = \operatorname{erfc}\frac{(2n+1)a\pm r}{2(Dt)^{1/2}}\,dr \, ,$$

which yields

$$f = \frac{3}{a^2}\left[a\sum_{n=0}^{\infty} 2(Dt)^{1/2}\, i\operatorname{erfc}\frac{(2n+1)a-a}{2(Dt)^{1/2}} - 4(Dt)\sum_{n=0}^{\infty} i^2\operatorname{erfc}\frac{(2n+1)a-a}{2(Dt)^{1/2}}\right.$$

$$\left. + a\sum_{n=0}^{\infty} 2(Dt)^{1/2}\, i\operatorname{erfc}\frac{(2n+1)a+a}{2(Dt)^{1/2}} + 4(Dt)\sum_{n=0}^{\infty} i^2\operatorname{erfc}\frac{(2n+1)a+a}{2(Dt)^{1/2}}\right] =$$

$$= 6\left(\frac{Dt}{a^2}\right)^{1/2}\left[\sum_{n=0}^{\infty} \text{ierfc}\,\frac{na}{(Dt)^{1/2}} + \sum_{n=0}^{\infty} \text{ierfc}\,\frac{(n+1)a}{(Dt)^{1/2}}\right] \qquad \text{(B-35)}$$

$$- 12\left(\frac{Dt}{a^2}\right)\left[\sum_{n=0}^{\infty} i^2\text{erfc}\,\frac{na}{(Dt)^{1/2}} - \sum_{n=0}^{\infty} i^2\text{erfc}\,\frac{(n+1)a}{(Dt)^{1/2}}\right].$$

By letting $n + 1 = m$, the ierfc terms may be combined; the i^2erfc terms will cancel except for an i^2erfc 0 term. Noting that the ierfc $0 = \pi^{-1/2}$ and $i^2\text{erfc}\ 0 = 1/4$, one finds that Eq. (B-35) becomes

$$f = 6\left(\frac{Dt}{a^2}\right)^{1/2}\left[\pi^{-1/2} + 2\sum_{n=1}^{\infty} \text{ierfc}\,\frac{na}{(Dt)^{1/2}}\right] - 3\left(\frac{Dt}{a^2}\right). \qquad \text{(B-36)}$$

For $t \to 0$, the terms in Eq. (B-36) involving ierfc $k/t^{1/2}$ become zero. For $t = 0$, the remaining terms are zero; thus, the fractional release is zero.

If the substitution of Eq. (C-7) is made for ierfc $\frac{na}{\sqrt{Dt}}$ in Eq. (B-36), the resulting expression becomes

$$f = 6\left(\frac{Dt}{a^2}\right)^{1/2}\left[\pi^{-1/2} + 2\pi^{-1/2}\sum_{n=1}^{\infty} \exp\left(-\frac{n^2a^2}{Dt}\right) - 2\sum_{n=1}^{\infty} \frac{na}{(Dt)^{1/2}}\text{erfc}\,\frac{na}{(Dt)^{1/2}}\right] - 3\left(\frac{Dt}{a^2}\right). \qquad \text{(B-37)}$$

For large t, as $t \to \infty$, $\frac{1}{Dt} \to 0$; thus, Eq. (B-32) may be substituted into Eq. (B-37). Hence,

$$\lim_{t\to\infty} f = \lim_{t\to\infty}\left[6\left(\frac{Dt}{a^2}\right)^{1/2}\left\{\pi^{-1/2} - 2\sum_{n=1}^{\infty}\frac{na}{(Dt)^{1/2}}\text{erfc}\,\frac{na}{(Dt)^{1/2}} + \pi^{-1/2}\left[\frac{1}{a}(\pi Dt)^{1/2} - 1\right]\right\} - 3\left(\frac{Dt}{a^2}\right)\right]$$

$$= \lim_{t\to\infty}\left[-12\sum_{n=1}^{\infty}(n)\text{erfc}\,\frac{na}{(Dt)^{1/2}} + 6\left(\frac{Dt}{a^2}\right) - 3\left(\frac{Dt}{a^2}\right)\right] \qquad \text{(B-38)}$$

$$= \lim_{t\to\infty}\left[3\left(\frac{Dt}{a^2}\right) - 12\sum_{n=1}^{\infty}(n)\,\text{erfc}\,\frac{na}{(Dt)^{1/2}}\right].$$

This is equivalent to $\infty \to \infty$, which is indeterminate. Referring to Eq. (B-34), one finds for large values of t that the difference between the two complementary error functions may be approximated by

$$\frac{2}{\pi^{1/2}}\left[\frac{(2n+1)a+r}{2(Dt)^{1/2}}-\frac{(2n+1)a-r}{2(Dt)^{1/2}}\right]\exp\left[-\frac{(2n+1)^2a^2}{4Dt}\right]=\frac{2r}{(\pi Dt)^{1/2}}\exp\left[-\frac{(2n+1)^2a^2}{4Dt}\right],$$

which, upon substitution in Eq. (B-34), gives

$$\lim_{t\to\infty} f=\lim_{t\to\infty}\frac{3}{a^2}\int_0^a\frac{2r^2}{(\pi Dt)^{1/2}}\sum_{n=0}^{\infty}\exp\left[-\frac{(2n+1)^2a^2}{4Dt}\right]dr$$

$$=\lim_{t\to\infty}\frac{6}{a^2(\pi Dt)^{1/2}}\int_0^a r^2\left\{\sum_{n=1}^{\infty}\exp\left[-\frac{n^2a^2}{4Dt}\right]-\sum_{n=1}^{\infty}\exp\left[-\frac{(2n)^2a^2}{4Dt}\right]\right\}dr.$$

Applying Eq. (B-32), one finds

$$\lim_{t\to\infty} f=\lim_{t\to\infty}\frac{6}{a^2(\pi Dt)^{1/2}}\int_0^a r^2\left[\frac{1}{2a}(4\pi Dt)^{1/2}-\frac{1}{2a}(\pi Dt)^{1/2}\right]dr$$

$$=\lim_{t\to\infty}\frac{3}{a^3(\pi Dt)^{1/2}}\int_0^a r^2\left[2(\pi Dt)^{1/2}-(\pi Dt)^{1/2}\right]dr$$

$$=\frac{3}{a^3}\int_0^a r^2dr=\frac{3a^3}{3a^3}=1\,.$$

Thus,

$$\lim_{t\to\infty} f = 1\,. \qquad \text{(B-39)}$$

It has now been shown how Eqs. (B-6) and (B-8) were obtained, and it has further been demonstrated that the tracer concentration and the fractional release approach the proper limits for large periods of time and at time $t = 0$.

Booth has shown that for values of $\frac{\pi^2 Dt}{a^2} < 1$, Eqs. (B-7) and (B-8) are identical.[6]

Solutions of the form (B-7) converge slowly for small values of Dt/a^2, but solutions of the form (B-8) are rapidly convergent for the same small values.[7] This statement also applies to the equations for the tracer concentrations, i.e., to Eqs. (B-5) and (B-6).

C. Properties of the Error Function and Related Functions

The following definitions are made:[7]

$$\operatorname{erf} x = \frac{2}{\sqrt{\pi}} \int_0^x e^{-z^2}\, dz \,, \tag{C-1}$$

$$\operatorname{erf} \infty = 1 \,, \tag{C-2}$$

$$\operatorname{erf}(-x) = -\operatorname{erf} x \,, \tag{C-3}$$

$$\operatorname{erfc} x = 1 - \operatorname{erf} x = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-z^2}\, dz \,, \tag{C-4}$$

$$\operatorname{ierfc} x = \int_x^\infty \operatorname{erfc} z \, dz \,, \tag{C-5}$$

$$i^n\operatorname{erfc} x = \int_x^\infty i^{n-1} \operatorname{erfc} z \, dz \,, \tag{C-6}$$

where

$$i^0\operatorname{erfc} x = \operatorname{erfc} x \,, \tag{C-6a}$$

$$\operatorname{ierfc} x = \frac{1}{\sqrt{\pi}} e^{-x^2} - x \times \operatorname{erfc} x \,, \tag{C-7}$$

and

$$i^2\operatorname{erfc} x = \frac{1}{4}\left[\operatorname{erfc} x - 2x \operatorname{ierfc} x\right] . \tag{C-8}$$

The general recursion formula is

$$2n\, i^n\operatorname{erfc} x = i^{n-2}\operatorname{erfc} x - 2x\, i^{n-1}\operatorname{erfc} x \,. \tag{C-9}$$

If both sides of Eq. (C-6) are differentiated,

$$\begin{aligned} \frac{d}{dx}\, i^{n+1}\operatorname{erfc} z &= \frac{d}{dx} \int_z^\infty i^n\operatorname{erfc} y \, dy \\ &= -i^n\operatorname{erfc} z \frac{dz}{dx} \,. \end{aligned} \tag{C-10}$$

Integrating both sides of (C-10) and rearranging yields

$$\int i^n \text{erfc } z \, dx = -\frac{1}{\frac{dz}{dx}} \, i^{n+1} \text{erfc } z \qquad \text{(C-11)}$$

provided $\frac{dz}{dx}$ is a constant and the constant of integration is neglected; then (C-11) is the indefinite integral of i^nerfc z dx, where z is a function of x.

The values of i^nerfc(-x) will now be studied to obtain an inversion formula, so that the tabulated values of the positive argument may be used.

Noting

$$\text{erf}(-x) = -\text{erf } x \qquad \text{(C-3)}$$

and

$$\text{erfc } x = 1 - \text{erf } x \,, \qquad \text{(C-4)}$$

one obtains

$$\begin{aligned} \text{erfc}(-x) &= 1 - \text{erf}(-x) = 1 + \text{erf } x \\ &= 1 + (1 - \text{erfc } x) \qquad \text{(C-12)} \\ &= 2 - \text{erfc } x \,. \end{aligned}$$

Thus,

$$\text{ierfc } x = \frac{1}{\sqrt{\pi}} e^{-x^2} - x \text{ erfc } x \,, \qquad \text{(C-7)}$$

and

$$\begin{aligned} \text{ierfc}(-x) &= \frac{1}{\sqrt{\pi}} e^{-(-x)^2} - (-x)\text{erfc}(-x) \\ &= \frac{1}{\sqrt{\pi}} e^{-x^2} + x\text{erfc}(-x) \\ &= \frac{1}{\sqrt{\pi}} e^{-x^2} + x(2 - \text{erfc } x) \qquad \text{(C-13)} \\ &= 2x + \left[\frac{1}{\sqrt{\pi}} e^{-x^2} - x\text{erfc } x\right] \\ &= 2x + \text{ierfc } x \,. \end{aligned}$$

So,

$$i^2\text{erfc } x = \frac{1}{4} \left[\text{erfc } x - 2x \text{ ierfc } x\right] , \qquad \text{(C-8)}$$

and

$$\begin{aligned} i^2\mathrm{erfc}\,(-x) &= \frac{1}{4}\,[\mathrm{erfc}\,(-x)\ -2\,(-x)\ \mathrm{ierfc}\,(-x)] \\ &= \frac{1}{4}\,[(2-\mathrm{erfc}x) + 2x\,(2x+\mathrm{ierfc}\ x)\,] \\ &= \frac{1}{2} - \frac{1}{4}\,(\mathrm{erfc}\ x - 2x\ \mathrm{ierfc}\ x) + x^2 \\ &= \frac{1}{2} + x^2 - i^2\mathrm{erfc}\ x\,. \end{aligned} \tag{C-14}$$

By using the general recursion formula (C-9) and the relations just developed, it may be shown that succeeding terms are

$$i^3\mathrm{erfc}\,(-x) = \frac{1}{2}\,x + \frac{1}{3}\,x^3 + i^3\mathrm{erfc}\ x\,, \tag{C-15}$$

$$i^4\mathrm{erfc}\,(-x) = \frac{1}{16} + \frac{1}{4}\,x^2 + \frac{1}{12}\,x^4 - i^4\mathrm{erfc}\ x\,, \tag{C-16}$$

and

$$i^5\mathrm{erfc}\,(-x) = \frac{1}{16}\,x + \frac{1}{12}\,x^3 + \frac{1}{60}\,x^5 + i^5\mathrm{erfc}\ x\,. \tag{C-17}$$

From the foregoing, a general inversion formula for $i^n\mathrm{erfc}(-x)$ may be obtained:

$$\begin{aligned} i^n\mathrm{erfc}\,(-x) = (-1)^{n+1}\ i^n\mathrm{erfc}\ x + \frac{2x^n}{n\,!} + \frac{x^{n-2}}{2(n-2)!} \\ + \frac{x^{n-4}}{16(n-4)!} + \cdots + \frac{2x^{n-m}}{(4\cdot 8\cdot 12\cdots 2m)(n-m)!} \end{aligned} \tag{C-18}$$

where $n - m = 1$ for $n = 3, 5, 7, \cdots,$

and $n - m = 0$ for $n = 2, 4, 6, \cdots.$

D. Solution of the Slab Problem for a Moving Boundary

D.1. Concentration of the Tracer

An expression for the fractional release of a tracer element through the moving boundary of a slab will be obtained. Chambré[5] has derived a general solution for the tracer concentration for a slab $-(a - bt) < x < a - bt$ and $0 < t < \frac{a}{b}$, where b is the rate of movement of the boundary

$$C(x,t) = \frac{1}{2(\pi D t)^{1/2}} \left\{ \int_{-a}^{a} f(\xi) \exp\left[-\frac{(x-\xi)^2}{4Dt}\right] d\xi \right. \tag{D-1}$$
$$\left. + \sum_{n=1}^{\infty} (-1)^n \int_{-a}^{a} f(\xi) \exp\left[\frac{nb}{D}(\xi + na)\right] S(x,t;\xi+2na)\, d\xi \right\},$$

$$S(x,t;\xi) = \exp\left[-\frac{(x-\xi)^2}{4Dt}\right] + \exp\left[-\frac{(x+\xi)^2}{4Dt}\right]. \tag{D-1a}$$

This equation is the solution of the diffusion equation

$$\frac{\partial C(x,t)}{\partial t} = D\, \frac{\partial^2 C(x,t)}{\partial x^2}\,, \tag{D-2}$$

subject to the restricting conditions

$$C(x,0) = f(x) \quad \text{for} \quad 0 < x < a, \tag{D-2a}$$

$$\frac{\partial C(0,t)}{\partial x} = 0 \quad \text{for} \quad 0 < t < \frac{a}{b}, \tag{D-2b}$$

and

$$C(a-bt,t) = 0 \quad \text{for} \quad 0 < t < \frac{a}{b}. \tag{D-2c}$$

For this problem, the initial condition (D-2a) shall be assumed to be a constant, C_0; thus,

$$C(x,0) = C_0 \quad \text{for} \quad 0 < |x| < a. \tag{D-3}$$

If this substitution and $S(x, t; \xi + 2na)$ are made into Eq. (D-1), one has

$$C(x,t) = \frac{C_0}{2(\pi D t)^{1/2}} \left[\int_{-a}^{a} \exp\left[-\frac{(x-\xi)^2}{4Dt}\right] d\xi \; + \right.$$

$$+\int_{-a}^{a}\sum_{n=1}^{\infty}(-1)^n \exp\left[\frac{nb}{D}(\xi+na)\right]\left(\exp\left\{-\frac{[x-(\xi+2na)]^2}{4Dt}\right\}+\exp\left\{-\frac{[x+(\xi+2na)]^2}{4Dt}\right\}\right)d\xi\Bigg]. \qquad \text{(D-4)}$$

This may be simplified somewhat by defining

$$y = \xi + 2na \qquad \text{(D-5)}$$

and

$$z = \frac{x-\xi}{2\sqrt{Dt}}, \qquad \text{(D-6)}$$

upon which Eq. (D-4) becomes

$$C(x,t) = \frac{C_0}{2(\pi Dt)^{1/2}}\Bigg(-2(Dt)^{1/2}\int_{\frac{x+a}{2(Dt)^{1/2}}}^{\frac{x-a}{2(Dt)^{1/2}}} \exp(-z^2)\,dz$$

$$+\int_{a(2n-1)}^{a(2n+1)}\sum_{n=1}^{\infty}(-1)^n \exp\left[\frac{nb}{D}(y-na)\right]\left\{\exp\left[-\frac{(x-y)^2}{4Dt}\right]+\exp\left[-\frac{(x+y)^2}{4Dt}\right]\right\}dy\Bigg). \qquad \text{(D-7)}$$

The first term may now be integrated directly, and if exponentials are combined, one has

$$C(x,t) = \frac{C_0}{2}\left\{\operatorname{erf}\left[\frac{x+a}{2(Dt)^{1/2}}\right]-\operatorname{erf}\left[\frac{x-a}{2(Dt)^{1/2}}\right]\right\}$$

$$+\frac{C_0}{2(\pi Dt)^{1/2}}\left\{\sum_{n=1}^{\infty}(-1)^n \exp\left[-\frac{nb}{D}(na)\right]\int_{a(2n-1)}^{a(2n+1)}\left(\exp\left[-\frac{(x-y)^2}{4Dt}+\frac{nby}{D}\right]\right.\right. \qquad \text{(D-8)}$$

$$\left.\left.+\exp\left[-\frac{(x+y)^2}{4Dt}+\frac{nby}{D}\right]\right)dy\right\}.$$

The exponentials may be simplified,

$$\frac{(x-y)^2}{4Dt}-\frac{nby}{D} = \frac{1}{4Dt}\left\{x^2-2xy+y^2-4nbty\right\}$$

$$=\frac{1}{4Dt}\left\{y^2-2y(x+2nbt)+(x+2nbt)^2+x^2-(x+2nbt)^2\right\} =$$

$$\begin{aligned} &= \frac{1}{4Dt}\left\{\left[y-(x+2nbt)\right]^2 - 4nbt(x+nbt)\right\} \\ &= \frac{1}{4Dt}\left[y-(x+2nbt)\right]^2 - \frac{nb}{D}(x+nbt); \end{aligned} \tag{D-9a}$$

$$\begin{aligned} \frac{(x+y)^2}{4Dt} - \frac{nby}{D} &= \frac{1}{4Dt}\left\{x^2+2xy+y^2-4nbty\right\} \\ &= \frac{1}{4Dt}\left\{y^2+2y(x-2nbt)+(x-2nbt)^2+x^2-(x-2nbt)^2\right\} \\ &= \frac{1}{4Dt}\left\{\left[y+(x-2nbt)\right]^2 + 4nbt(x-nbt)\right\} \\ &= \frac{1}{4Dt}\left[y+(x-2nbt)\right]^2 + \frac{nb}{D}(x-nbt); \end{aligned} \tag{D-9b}$$

$$\begin{aligned} C(x,t) &= \frac{C_0}{2}\left[\operatorname{erf}\frac{x+a}{2(Dt)^{1/2}} - \operatorname{erf}\frac{x-a}{2(Dt)^{1/2}}\right] \\ &+ \frac{C_0}{2(\pi Dt)^{1/2}}\sum_{n=1}^{\infty}(-1)^n \exp\left[-\frac{nb}{D}(na-nbt-x)\right]\int_{a(2n-1)}^{a(2n+1)} \exp\left\{-\frac{\left[y-(x+2nbt)\right]^2}{4Dt}\right\}dy \\ &+ \frac{C_0}{2(\pi Dt)^{1/2}}\sum_{n=1}^{\infty}(-1)^n \exp\left[-\frac{nb}{D}(na-nbt+x)\right]\int_{a(2n-1)}^{a(2n+1)} \exp\left\{-\frac{\left[y+(x-2nbt)\right]^2}{4Dt}\right\}dy\,. \end{aligned} \tag{D-10}$$

Simple substitutions similar to Eq. (D-6) allow the last two terms of Eq. (D-10) to be integrated:

$$\begin{aligned}C(x,t) &= \frac{C_0}{2}\left[\operatorname{erf}\frac{x+a}{2(Dt)^{1/2}} - \operatorname{erf}\frac{x-a}{2(Dt)^{1/2}}\right]\\ &+ \frac{C_0}{2}\sum_{n=1}^{\infty}(-1)^n \exp\left[-\frac{nb}{D}(na-nbt-x)\right]\left[\operatorname{erf}\frac{a(2n+1)-(x+2nbt)}{2(Dt)^{1/2}}\right.\\ &\qquad\qquad\left. - \operatorname{erf}\frac{a(2n-1)-(x+2nbt)}{2(Dt)^{1/2}}\right]\\ &+ \frac{C_0}{2}\sum_{n=1}^{\infty}(-1)^n \exp\left[-\frac{nb}{D}(na-nbt+x)\right]\left[\operatorname{erf}\frac{a(2n+1)+(x-2nbt)}{2(Dt)^{1/2}}\right.\\ &\qquad\qquad\left. - \operatorname{erf}\frac{a(2n-1)+(x-2nbt)}{2(Dt)^{1/2}}\right].\end{aligned} \tag{D-11}$$

Using Eq. (C-3) and rearranging terms, one has

$$\begin{aligned}C(x,t) &= \frac{C_0}{2}\left[\operatorname{erf}\frac{a+x}{2(Dt)^{1/2}} + \operatorname{erf}\frac{a-x}{2(Dt)^{1/2}}\right]\\ &+ \frac{C_0}{2}\sum_{n=1}^{\infty}(-1)^n \exp\left[-\frac{nb}{D}(na-nbt-x)\right]\left[\operatorname{erf}\frac{2n(a-bt)+a-x}{2(Dt)^{1/2}}\right.\\ &\qquad\qquad\left. - \operatorname{erf}\frac{2n(a-bt)-a-x}{2(Dt)^{1/2}}\right]\\ &+ \frac{C_0}{2}\sum_{n=1}^{\infty}(-1)^n \exp\left[-\frac{nb}{D}(na-nbt+x)\right]\left[\operatorname{erf}\frac{2n(a-bt)+a+x}{2(Dt)^{1/2}}\right.\\ &\qquad\qquad\left. - \operatorname{erf}\frac{2n(a-bt)-a+x}{2(Dt)^{1/2}}\right].\end{aligned} \tag{D-12}$$

With the use of Eq. (C-4), i. e., erfc $x = 1 - \operatorname{erf} x$, one finds

$$\begin{aligned}C(x,t) &= C_0 - \frac{C_0}{2}\left[\operatorname{erfc}\frac{a+x}{2(Dt)^{1/2}} + \operatorname{erfc}\frac{a-x}{2(Dt)^{1/2}}\right]\\ &+ \frac{C_0}{2}\sum_{n=1}^{\infty}(-1)^n \exp\left[-\frac{nb}{D}(na-nbt-x)\right]\left[\operatorname{erfc}\frac{2n(a-bt)-a-x}{2(Dt)^{1/2}}\right.\\ &\qquad\qquad\left. - \operatorname{erfc}\frac{2n(a-bt)+a-x}{2(Dt)^{1/2}}\right]\\ &+ \frac{C_0}{2}\sum_{n=1}^{\infty}(-1)^n \exp\left[-\frac{nb}{D}(na-nbt+x)\right]\left[\operatorname{erfc}\frac{2n(a-bt)-a+x}{2(Dt)^{1/2}}\right.\\ &\qquad\qquad\left. - \operatorname{erfc}\frac{2n(a-bt)+a+x}{2(Dt)^{1/2}}\right].\end{aligned} \tag{D-13}$$

For $t = 0$, because erfc $\infty = 0$, Eq. (D-13) becomes

$$C(x, 0) = C_0 .$$

For $t = a/b$, which corresponds to total evaporation, the tracer concentration should become zero. Hence,

$$\begin{aligned} C\left(x,\frac{a}{b}\right) &= C_0 - \frac{C_0}{2}\left[\operatorname{erfc}\frac{a+x}{2\left(\frac{Da}{b}\right)^{1/2}} + \operatorname{erfc}\frac{a-x}{2\left(\frac{Da}{b}\right)^{1/2}}\right] \\ &+ \frac{C_0}{2}\sum_{n=1}^{\infty}(-1)^n \exp\left(\frac{nbx}{D}\right)\left[\operatorname{erfc}\frac{-(a+x)}{2\left(\frac{Da}{b}\right)^{1/2}} - \operatorname{erfc}\frac{a-x}{2\left(\frac{Da}{b}\right)^{1/2}}\right] \\ &+ \frac{C_0}{2}\sum_{n=1}^{\infty}(-1)^n \exp\left(-\frac{nbx}{D}\right)\left[\operatorname{erfc}\frac{-a+x}{2\left(\frac{Da}{b}\right)^{1/2}} - \operatorname{erfc}\frac{a+x}{2\left(\frac{Da}{b}\right)^{1/2}}\right] . \end{aligned} \tag{D-14}$$

Since $|x| < a - bt$ at $t = a/b$, x in Eq. (D-14) must be zero. Thus,

$$\begin{aligned} C\left(x,\frac{a}{b}\right) &= C_0 - \frac{C_0}{2}\left[2\operatorname{erfc}\left(\frac{ba}{4D}\right)^{1/2}\right] + \frac{C_0}{2}\sum_{n=1}^{\infty}(-1)^n\left\{2\operatorname{erfc}\left[-\frac{1}{2}\left(\frac{ba}{D}\right)^{1/2}\right] - 2\operatorname{erfc}\left[\frac{1}{2}\left(\frac{ba}{D}\right)^{1/2}\right]\right\}, \\ &= C_0 - C_0\operatorname{erfc}\left[\frac{1}{2}\left(\frac{ba}{D}\right)^{1/2}\right] + C_0\sum_{n=1}^{\infty}(-1)^n\left\{\operatorname{erfc}\left[\frac{-1}{2}\left(\frac{ba}{D}\right)^{1/2}\right] - \operatorname{erfc}\left[\frac{1}{2}\left(\frac{ba}{D}\right)^{1/2}\right]\right\} \end{aligned}$$

with the use of Eq. (C-12),

$$= C_0\left[1 - \operatorname{erfc}\frac{1}{2}\left(\frac{ba}{D}\right)^{1/2}\right] + 2C_0\sum_{n=1}^{\infty}(-1)^n\left[1 - \operatorname{erfc}\frac{1}{2}\left(\frac{ba}{D}\right)^{1/2}\right] . \tag{D-15}$$

It was previously shown in Eq. (A-41) that $2\sum_{n=0}^{\infty}(-1)^n = 1$; similarly, it can be shown that $2\sum_{n=1}^{\infty}(-1)^n = -1$. With this substitution, Eq. (D-15) is

$$C\left(x,\frac{a}{b}\right) = C_0\left[1 - \operatorname{erfc}\frac{1}{2}\left(\frac{ba}{D}\right)^{1/2}\right] - C_0\left[1 - \operatorname{erfc}\frac{1}{2}\left(\frac{ba}{D}\right)^{1/2}\right] = 0 . \tag{D-16}$$

If, in Eq. (D-13), $b = 0$, which corresponds to no evaporation, then

$$C(x,t) = C_0 - \frac{C_0}{2}\left[\operatorname{erfc}\frac{a+x}{2(Dt)^{1/2}} + \operatorname{erfc}\frac{a-x}{2(Dt)^{1/2}}\right]$$

$$+ \frac{C_0}{2}\sum_{n=1}^{\infty}(-1)^n\left[\operatorname{erfc}\frac{(2n-1)a-x}{2(Dt)^{1/2}} - \operatorname{erfc}\frac{(2n+1)a-x}{2(Dt)^{1/2}}\right. \tag{D-17}$$

$$\left. + \operatorname{erfc}\frac{(2n-1)a+x}{2(Dt)^{1/2}} - \operatorname{erfc}\frac{(2n+1)a+x}{2(Dt)^{1/2}}\right].$$

If $2n - 1 = 2m + 1$, Eq. (D-17) becomes

$$C(x,t) = C_0 - \frac{C_0}{2}\left[\operatorname{erfc}\frac{a+x}{2(Dt)^{1/2}} + \operatorname{erfc}\frac{a-x}{2(Dt)^{1/2}}\right] - \frac{C_0}{2}\sum_{n=1}^{\infty}(-1)^n\left[\operatorname{erfc}\frac{(2n+1)a+x}{2(Dt)^{1/2}}\right.$$

$$\left. + \operatorname{erfc}\frac{(2n+1)a-x}{2(Dt)^{1/2}}\right] + \frac{C_0}{2}\sum_{m=0}^{\infty}(-1)^{m+1}\left[\operatorname{erfc}\frac{(2m+1)a+x}{2(Dt)^{1/2}} + \operatorname{erfc}\frac{(2m+1)a-x}{2(Dt)^{1/2}}\right]$$

$$= C_0 - \frac{C_0}{2}\sum_{n=0}^{\infty}(-1)^n\left[\operatorname{erfc}\frac{(2n+1)a+x}{2(Dt)^{1/2}} + \operatorname{erfc}\frac{(2n+1)a-x}{2(Dt)^{1/2}}\right] \tag{D-18}$$

$$- \frac{C_0}{2}\sum_{m=0}^{\infty}(-1)^m\left[\operatorname{erfc}\frac{(2m+1)a+x}{2(Dt)^{1/2}} + \operatorname{erfc}\frac{(2m+1)a-x}{2(Dt)^{1/2}}\right]$$

$$= C_0 - C_0\sum_{n=0}^{\infty}(-1)^n\left[\operatorname{erfc}\frac{(2n+1)a-x}{2(Dt)^{1/2}} + \operatorname{erfc}\frac{(2n+1)a+x}{2(Dt)^{1/2}}\right],$$

which may be recognized as Eq. (A-6).

D.2. Fractional Release of the Tracer

The fractional release may be computed from Eq. (A-17), as follows:

$$f = \frac{Q_0 - Q(t)}{Q_0} = \frac{2aC_0 - \int_{-(a-bt)}^{(a-bt)} C(x,t)\,dx}{2aC_0} =$$

$$= 1-\frac{1}{2aC_0}\int_{-(a-bt)}^{(a-bt)} C(x,t)\,dx\ ;$$

using the symmetry relation, one obtains

$$f = 1-\frac{1}{aC_0}\int_{0}^{(a-bt)} C(x,t)\,dx\,. \tag{D-19}$$

With the substitution of Eq (D-13) for C(x, t), it follows that

$$\begin{aligned} f = 1 &- \frac{1}{aC_0}\int_0^{(a-bt)} C_0\,dx + \frac{1}{aC_0}\int_0^{(a-bt)} \frac{C_0}{2}\left[\operatorname{erfc}\frac{a+x}{2(Dt)^{1/2}} + \operatorname{erfc}\frac{a-x}{2(Dt)^{1/2}}\right]dx \\ &- \frac{1}{aC_0}\int_0^{(a-bt)} \frac{C_0}{2}\sum_{n=1}^{\infty}(-1)^n \exp\left[-\frac{nb}{D}(na-nbt-x)\right]\left[\operatorname{erfc}\frac{2n(a-bt)-a-x}{2(Dt)^{1/2}}\right. \\ &\qquad\qquad \left. - \operatorname{erfc}\frac{2n(a-bt)+a-x}{2(Dt)^{1/2}}\right]dx \\ &- \frac{1}{aC_0}\int_0^{(a-bt)} \frac{C_0}{2}\sum_{n=1}^{\infty}(-1)^n \exp\left[-\frac{nb}{D}(na-nbt+x)\right]\left[\operatorname{erfc}\frac{2n(a-bt)-a+x}{2(Dt)^{1/2}}\right. \\ &\qquad\qquad \left. - \operatorname{erfc}\frac{2n(a-bt)+a+x}{2(Dt)^{1/2}}\right]dx. \end{aligned} \tag{D-20}$$

With the use of Eq. (C-11) in the second integral, Eq. (D-20) becomes

$$\begin{aligned} f = \frac{bt}{a} &+ \frac{(Dt)^{1/2}}{a}\left[-i\operatorname{erfc}\frac{2a-bt}{2(Dt)^{1/2}} + i\operatorname{erfc}\frac{a}{2(Dt)^{1/2}} + i\operatorname{erfc}\frac{bt}{2(Dt)^{1/2}} - i\operatorname{erfc}\frac{a}{2(Dt)^{1/2}}\right] \\ &- \frac{1}{2a}\sum_{n=1}^{\infty}(-1)^n \exp\left[-\frac{nb}{D}(n)(a-bt)\right]\int_0^{(a-bt)} \exp\left(\frac{nbx}{D}\right)\left[\operatorname{erfc}\frac{2n(a-bt)-a-x}{2(Dt)^{1/2}}\right. \\ &\qquad\qquad \left. - \operatorname{erfc}\frac{2n(a-bt)+a-x}{2(Dt)^{1/2}}\right]dx \\ &- \frac{1}{2a}\sum_{n=1}^{\infty}(-1)^n \exp\left[-\frac{nb}{D}(n)(a-bt)\right]\int_0^{(a-bt)} \exp\left(-\frac{nbx}{D}\right)\left[\operatorname{erfc}\frac{2n(a-bt)-a+x}{2(Dt)^{1/2}}\right. \\ &\qquad\qquad \left. - \operatorname{erfc}\frac{2n(a-bt)+a+x}{2(Dt)^{1/2}}\right]dx = \end{aligned}$$

$$= \frac{bt}{a} + \left(\frac{Dt}{a^2}\right)^{1/2} \left[i\,\mathrm{erfc}\,\frac{bt}{2(Dt)^{1/2}} - i\,\mathrm{erfc}\,\frac{2a-bt}{2(Dt)^{1/2}} \right] \tag{D-21}$$

$$- \frac{1}{2a} \sum_{n=1}^{\infty} (-1)^n \exp\left[-\frac{nb}{D}(n)(a-bt)\right] \left\{ \int_0^{(a-bt)} \exp\left(\frac{nbx}{D}\right) \left[\mathrm{erfc}\,\frac{2n(a-bt)-a-x}{2(Dt)^{1/2}} \right. \right.$$

$$\left. \left. - \mathrm{erfc}\,\frac{2n(a-bt)+a-x}{2(Dt)^{1/2}} \right] dx + \int_0^{(a-bt)} \exp\left(-\frac{nbx}{D}\right) \left[\mathrm{erfc}\,\frac{2n(a-bt)-a+x}{2(Dt)^{1/2}} - \mathrm{erfc}\,\frac{2n(a-bt)+a+x}{2(Dt)^{1/2}} \right] dx \right\}.$$

The remaining integrals in the expression (D-21) for f may be evaluated by integrating by parts, as follows. Let

$u = \exp\left(\frac{nbx}{D}\right)$ and $dv = \mathrm{erfc}\,\frac{2n(a-bt) \pm a - x}{2(Dt)^{1/2}}\,dx$; then

$du = \frac{nb}{D} \exp\left(\frac{nbx}{D}\right) dx$ and $v = 2(Dt)^{1/2}\, i\,\mathrm{erfc}\,\frac{2n(a-bt) \pm a - x}{2(Dt)^{1/2}}$.

The result may be written as

$$2(Dt)^{1/2} \sum_{m=1}^{\infty} (-1)^{m+1} \exp\left(\frac{nbx}{D}\right) \left[2\left(\frac{nb}{D}\right)(Dt)^{1/2} \right]^{m-1} i^m \mathrm{erfc}\,\frac{2n(a-bt) \pm a - x}{2(Dt)^{1/2}} \,. \tag{D-22}$$

To integrate the second integral by parts, let

$u = \exp\left(-\frac{nbx}{D}\right)$ and $dv = \mathrm{erfc}\,\frac{2n(a-bt) \pm a + x}{2(Dt)^{1/2}}\,dx$; then

$du = -\frac{nb}{D} \exp\left(-\frac{nbx}{D}\right) dx$ and $v = -2(Dt)^{1/2}\, i\,\mathrm{erfc}\,\frac{2n(a-bt) \pm a + x}{2(Dt)^{1/2}}$.

The result is

$$-2(Dt)^{1/2}\sum_{m=1}^{\infty}(-1)^{m+1}\exp\left(-\frac{nbx}{D}\right)\left[2\left(\frac{nb}{D}\right)(Dt)^{1/2}\right]^{m-1} i^m\operatorname{erfc}\frac{2n(a-bt)\pm a+x}{2(Dt)^{1/2}} \;. \tag{D-23}$$

Upon applying the limits to Eqs. (D-22) and (D-23) and inserting the results into Eq. (D-21), one obtains

$$\begin{aligned}
f = {} & \frac{bt}{a}+\left(\frac{Dt}{a^2}\right)^{1/2}\left[i\operatorname{erfc}\frac{bt}{2(Dt)^{1/2}}-i\operatorname{erfc}\frac{2a-bt}{2(Dt)^{1/2}}\right] \\
& -\left(\frac{Dt}{a^2}\right)^{1/2}\sum_{n=1}^{\infty}(-1)^n\exp\left[-\frac{nb}{D}(n)(a-bt)\right]\sum_{m=1}^{\infty}(-1)^{m+1}\left[2\left(\frac{nb}{D}\right)(Dt)^{1/2}\right]^{m-1}\left\{\exp\left[\frac{nb}{D}(a-bt)\right]i^m\operatorname{erfc}\frac{(2n-1)(a-bt)-a}{2(Dt)^{1/2}}\right. \\
& -i^m\operatorname{erfc}\frac{2n(a-bt)-a}{2(Dt)^{1/2}}-\exp\left[\frac{nb}{D}(a-bt)\right]i^m\operatorname{erfc}\frac{(2n-1)(a-bt)+a}{2(Dt)^{1/2}} \\
& +i^m\operatorname{erfc}\frac{2n(a-bt)+a}{2(Dt)^{1/2}}-\exp\left[-\frac{nb}{D}(a-bt)\right]i^m\operatorname{erfc}\frac{(2n+1)(a-bt)-a}{2(Dt)^{1/2}} \\
& \left.+i^m\operatorname{erfc}\frac{2n(a-bt)-a}{2(Dt)^{1/2}}+\exp\left[-\frac{nb}{D}(a-bt)\right]i^m\operatorname{erfc}\frac{(2n+1)(a-bt)+a}{2(Dt)^{1/2}}-i^m\operatorname{erfc}\frac{2n(a-bt)+a}{2(Dt)^{1/2}}\right\}.
\end{aligned} \tag{D-24}$$

After eliminating equal and opposite terms and combining exponentials, it follows that

$$\begin{aligned}
f = {} & \frac{bt}{a}+\left(\frac{Dt}{a^2}\right)^{1/2}\left[i\operatorname{erfc}\frac{bt}{2(Dt)^{1/2}}-i\operatorname{erfc}\frac{2a-bt}{2(Dt)^{1/2}}\right] \\
& -\left(\frac{Dt}{a^2}\right)^{1/2}\sum_{n=1}^{\infty}(-1)^n\exp\left[-\frac{nb}{n}(n)(a-bt)\right]\sum_{m=1}^{\infty}(-1)^{m+1}\left[2\left(\frac{nb}{D}\right)(Dt)^{1/2}\right]^{m-1}\left\{\exp\left[\frac{nb}{D}(a-bt)\right]i^m\operatorname{erfc}\frac{(2n-1)(a-bt)-a}{2(Dt)^{1/2}}\right. \\
& -\exp\left[\frac{nb}{D}(a-bt)\right]i^m\operatorname{erfc}\frac{(2n-1)(a-bt)+a}{2(Dt)^{1/2}}+\exp\left[-\frac{nb}{D}(a-bt)\right]i^m\operatorname{erfc}\frac{(2n+1)(a-bt)+a}{2(Dt)^{1/2}} \; -
\end{aligned}$$

$$- \exp\left[-\frac{nb}{D}(a-bt)\right] i^m\operatorname{erfc}\frac{(2n+1)(a-bt)-a}{2(Dt)^{1/2}} \tag{D-25}$$

$$= \frac{bt}{a} + \left(\frac{Dt}{a^2}\right)^{1/2}\left[\operatorname{ierfc}\frac{bt}{2(Dt)^{1/2}} - \operatorname{ierfc}\frac{2a-bt}{2(Dt)^{1/2}}\right]$$

$$+ \left(\frac{Dt}{a^2}\right)^{1/2}\sum_{n,m=1}^{\infty}(-1)^{n+m}\left[2\left(\frac{nb}{D}\right)(Dt)^{1/2}\right]^{m-1}\exp\left[-\frac{nb}{D}(n-1)(a-bt)\right]\left\{i^m\operatorname{erfc}\frac{(2n-1)(a-bt)-a}{2(Dt)^{1/2}} - i^m\operatorname{erfc}\frac{(2n-1)(a-bt)+a}{2(Dt)^{1/2}}\right\}$$

$$+ \left(\frac{Dt}{a^2}\right)^{1/2}\sum_{n,m=1}^{\infty}(-1)^{n+m}\left[2\left(\frac{nb}{D}\right)(Dt)^{1/2}\right]^{m-1}\exp\left[-\frac{nb}{D}(n+1)(a-bt)\right]\left\{i^m\operatorname{erfc}\frac{(2n+1)(a-bt)+a}{2(Dt)^{1/2}} - i^m\operatorname{erfc}\frac{(2n+1)(a-bt)-a}{2(Dt)^{1/2}}\right\}.$$

At $t=0$, each term of Eq. (D-25) becomes zero; thus, the fractional release is zero. At time, $t=a/b$, which corresponds to complete evaporation of the solid, the fractional release should be 1, as shown:

$$f = 1 + \left(\frac{D}{ab}\right)^{1/2}\left[\operatorname{ierfc}\frac{a}{2\left(\frac{Da}{b}\right)^{1/2}} - \operatorname{ierfc}\frac{2a-a}{2\left(\frac{Da}{b}\right)^{1/2}}\right]$$

$$+ \left(\frac{D}{ab}\right)^{1/2}\sum_{n,m=1}^{\infty}(-1)^{n+m}\left[2\left(\frac{nb}{D}\right)\left(\frac{Da}{b}\right)^{1/2}\right]^{m-1}\left\{i^m\operatorname{erfc}\frac{-a}{2\left(\frac{Da}{b}\right)^{1/2}} \right. \tag{D-26}$$

$$\left. - i^m\operatorname{erfc}\frac{a}{2\left(\frac{Da}{b}\right)^{1/2}} + i^m\operatorname{erfc}\frac{a}{2\left(\frac{Da}{b}\right)^{1/2}} - i^m\operatorname{erfc}\frac{-a}{2\left(\frac{Da}{b}\right)^{1/2}}\right\}$$

$$= 1.$$

If, in Eq. (D-25), b is set equal to zero, which corresponds to no evaporation, then

$$f = \left(\frac{Dt}{a^2}\right)^{1/2}\left[\operatorname{ierfc} 0 - \operatorname{ierfc}\frac{a}{(Dt)^{1/2}}\right] + \left(\frac{Dt}{a^2}\right)^{1/2}\sum_{n=1}^{\infty}(-1)^{n+1}\left[\operatorname{ierfc}\frac{(n-1)a}{(Dt)^{1/2}} \right. \tag{D-27}$$

$$\left. - \operatorname{ierfc}\frac{na}{(Dt)^{1/2}} + \operatorname{ierfc}\frac{(n+1)a}{(Dt)^{1/2}} - \operatorname{ierfc}\frac{na}{(Dt)^{1/2}}\right];$$

by letting $n - 1 = p$ and $n + 1 = m$ in Eq. (D-27), one obtains

$$f = \left(\frac{Dt}{a^2}\right)^{1/2}\Big[\text{ierfc } 0 - \text{ierfc } \frac{a}{(Dt)^{1/2}} + 2\sum_{n=1}^{\infty}(-1)^n \text{ierfc } \frac{na}{(Dt)^{1/2}}$$

$$+\sum_{m=2}^{\infty}(-1)^m \text{ierfc } \frac{ma}{(Dt)^{1/2}} + \sum_{p=0}^{\infty}(-1)^{p+2} \text{ierfc } \frac{pa}{(Dt)^{1/2}}\Big] \qquad \text{(D-28)}$$

$$= \left(\frac{Dt}{a^2}\right)^{1/2}\Big[2 \text{ ierfc } 0 + 2\sum_{n=1}^{\infty}(-1)^n \text{ierfc } \frac{na}{(Dt)^{1/2}}$$

$$+\sum_{m=1}^{\infty}(-1)^m \text{ierfc } \frac{ma}{(Dt)^{1/2}} + \sum_{p=1}^{\infty}(-1)^{p} \text{ierfc } \frac{pa}{(Dt)^{1/2}}\Big].$$

Noting that $\text{ierfc } 0 = \pi^{-1/2}$, and combining the m and p terms, one finds

$$f = 2\left(\frac{Dt}{a^2}\right)^{1/2}\Big[\pi^{-1/2} + 2\sum_{n=1}^{\infty}(-1)^n \text{ierfc } \frac{na}{(Dt)^{1/2}}\Big], \qquad \text{(D-29)}$$

which may be recognized as Eq. (A-8).

D.3. Conversion to Dimensionless Form

If one defines

$$\tau = \frac{Dt}{a^2} \qquad \text{(D-30)}$$

and

$$\beta = \frac{ba}{D}, \qquad \text{(D-31)}$$

so that

$$\beta\tau - \frac{ba}{D}\,\frac{Dt}{a^2} - \frac{bt}{a}, \qquad 0 < \beta\tau < 1, \qquad \text{(D-32)}$$

where $\beta\tau = 0$ corresponds to $t = 0$, and $\beta\tau = 1$ corresponds to complete evaporation, then Eq. (D-13) becomes

$$C\left(\frac{x}{a}, \tau\right) = C_0 - \frac{C_0}{2}\left(\text{erfc } \frac{1 + x/a}{2\tau^{1/2}} + \text{erfc } \frac{1 - x/a}{2\tau^{1/2}}\right) +$$

$$+\frac{C_0}{2}\sum_{n=1}(-1)^n\exp\left\{-n\beta\left[n(1-\beta\tau)-\frac{x}{a}\right]\right\}\left[\operatorname{erfc}\frac{2n(1-\beta\tau)-1-\frac{x}{a}}{2\tau^{1/2}}-\operatorname{erfc}\frac{2n(1-\beta\tau)+1-\frac{x}{a}}{2\tau^{1/2}}\right] \tag{D-33}$$

$$+\frac{C_0}{2}\sum_{n=1}^{\infty}(-1)^n\exp\left\{-n\beta\left[n(1-\beta\tau)+\frac{x}{a}\right]\right\}\left[\operatorname{erfc}\frac{2n(1-\beta\tau)-1+\frac{x}{a}}{2\tau^{1/2}}-\operatorname{erfc}\frac{2n(1-\beta\tau)+1+\frac{x}{a}}{2\tau^{1/2}}\right].$$

Equation (D-25) becomes

$$f=\beta\tau+\tau^{1/2}\left(i\operatorname{erfc}\frac{\beta\tau}{2\tau^{1/2}}-i\operatorname{erfc}\frac{2-\beta\tau}{2\tau^{1/2}}\right)$$

$$+\tau^{1/2}\sum_{n,m=1}^{\infty}(-1)^{n+m}(2n\beta\tau^{1/2})^{m-1}\exp[-n\beta(n-1)(1-\beta\tau)]\left[i^m\operatorname{erfc}\frac{(2n-1)(1-\beta\tau)-1}{2\tau^{1/2}}-i^m\operatorname{erfc}\frac{(2n-1)(1-\beta\tau)+1}{2\tau^{1/2}}\right] \tag{D-34}$$

$$+\tau^{1/2}\sum_{n,m=1}^{\infty}(-1)^{n+m}(2n\beta\tau^{1/2})^{m-1}\exp[-n\beta(n+1)(1-\beta\tau)]\left[i^m\operatorname{erfc}\frac{(2n+1)(1-\beta\tau)+1}{2\tau^{1/2}}-i^m\operatorname{erfc}\frac{(2n+1)(1-\beta\tau)-1}{2\tau^{1/2}}\right],$$

and Eq. (D-29) becomes

$$f=2\tau^{1/2}\left[\pi^{-1/2}+2\sum_{n=1}^{\infty}(-1)^n\,i\operatorname{erfc}\frac{n}{\tau^{1/2}}\right]. \tag{D-25}$$

D.4. Approximate Solution for the Fractional Release

If Eq. (D-34) is expanded to the first few terms in n, then

$$f=\beta\tau+\tau^{1/2}\left(i\operatorname{erfc}\frac{\beta\tau}{2\tau^{1/2}}-i\operatorname{erfc}\frac{2-\beta\tau}{2\tau^{1/2}}\right)$$

$$-\tau^{1/2}\sum_{m=1}^{\infty}(-1)^m(2\beta\tau^{1/2})^{m-1}\left(i^m\operatorname{erfc}\frac{-\beta\tau}{2\tau^{1/2}}-i^m\operatorname{erfc}\frac{2-\beta\tau}{2\tau^{1/2}}\right)-$$

$$-\tau^{1/2}\sum_{m=1}^{\infty}(-1)^m(2\beta\tau^{1/2})^{m-1}\exp[-2\beta(1-\beta\tau)]\left(i^m\text{erfc}\,\frac{4-3\beta\tau}{2\tau^{1/2}}-i^m\text{erfc}\,\frac{2-3\beta\tau}{2\tau^{1/2}}\right)$$

$$+\tau^{1/2}\sum_{m=1}^{\infty}(-1)^m(4\beta\tau^{1/2})^{m-1}\exp[-2\beta(1-\beta\tau)]\left(i^m\text{erfc}\,\frac{2-3\beta\tau}{2\tau^{1/2}}-i^m\text{erfc}\,\frac{4-3\beta\tau}{2\tau^{1/2}}\right) \quad \text{(D-36)}$$

$$+\tau^{1/2}\sum_{m=1}^{\infty}(-1)^m(4\beta\tau^{1/2})^{m-1}\exp[-6\beta(1-\beta\tau)]\left(i^m\text{erfc}\,\frac{6-5\beta\tau}{2\tau^{1/2}}-i^m\text{erfc}\,\frac{4-5\beta\tau}{2\tau^{1/2}}\right)$$

$$-\tau^{1/2}\sum_{m=1}^{\infty}(-1)^m(6\beta\tau^{1/2})^{m-1}\exp[-6\beta(1-\beta\tau)]\left(i^m\text{erfc}\,\frac{4-5\beta\tau}{2\tau^{1/2}}-i^m\text{erfc}\,\frac{6-5\beta\tau}{2\tau^{1/2}}\right)$$

$$-\tau^{1/2}\sum_{m=1}^{\infty}(-1)^m(6\beta\tau^{1/2})^{m-1}\exp[-12\beta(1-\beta\tau)]\left(i^m\text{erfc}\,\frac{8-7\beta\tau}{2\tau^{1/2}}-i^m\text{erfc}\,\frac{6-7\beta\tau}{2\tau^{1/2}}\right)$$

$$+\cdots.$$

Now, if the restrictions $\frac{Dt}{a^2} < 0.01$ and $\beta\tau < 0.5$ are made, then Eq. (D-36) may be closely approximated by

$$f=\beta\tau+\tau^{1/2}\,i\text{erfc}\,\frac{\beta\tau^{1/2}}{2}-\tau^{1/2}\sum_{m=1}^{\infty}(-1)^m(4)^{m-1}\left(\frac{\beta\tau^{1/2}}{2}\right)^{m-1}i^m\text{erfc}\,\frac{-\beta\tau^{1/2}}{2}\ . \quad \text{(D-37)}$$

Inversion formulae for $i^m\text{erfc}\,(-x)$ have been developed in Appendix C. If these are applied to Eq. (D-37) and expanded in terms of m, it can be seen, if sufficient terms are taken, that terms of $\left(\frac{\beta\tau^{1/2}}{2}\right)^x$ cancel and only the $i^m\text{erfc}\,\frac{\beta\tau^{1/2}}{2}$ terms are left. Thereupon the approximate expression for the fractional release, f, becomes

$$f=\beta\tau+2\tau^{1/2}\,i\text{erfc}\,\frac{\beta\tau^{1/2}}{2}+\sum_{m=1}^{\infty}(4)^m\left(\frac{\beta\tau^{1/2}}{2}\right)^m i^{m+1}\text{erfc}\,\frac{\beta\tau^{1/2}}{2}\ . \quad \text{(D-38)}$$

E. Solution of the Sphere Problem for a Moving Boundary

E.1. Concentration of the Tracer

In this section an expression for the fractional release of a tracer element through the moving boundary of a sphere is obtained. Chambré[5] has derived a general solution for the tracer concentration for a sphere $0 < r < a - bt$ and $0 < t < a/b$, where b is the rate of movement of the boundary

$$C(r,t) = \frac{1}{2r(\pi Dt)^{1/2}} \left\{ \int_{-a}^{a} \xi f(\xi) \exp\left[-\frac{(r-\xi)^2}{4Dt}\right] d\xi \right.$$

$$\left. + \sum_{n=1}^{\infty} \int_{-a}^{a} \xi f(\xi) \exp\left[\frac{nb}{D}(\xi+na)\right] S(r,t;\xi+2na)\, d\xi \right\} . \tag{E-1}$$

$$\text{and } S(r,t;\xi) = \exp\left[-\frac{(r-\xi)^2}{4Dt}\right] - \exp\left[-\frac{(r+\xi)^2}{4Dt}\right] . \tag{E-1a}$$

This equation is the solution to the diffusion equation

$$\frac{\partial C(r,t)}{\partial t} = D\left[\frac{\partial^2 C(r,t)}{\partial r^2} + \frac{2}{r}\frac{\partial C(r,t)}{\partial r}\right] \tag{E-2}$$

subject to the restricting conditions

$$C(r, 0) = f(r) \quad \text{for} \quad 0 < r < a , \tag{E-2a}$$

$$C(0, t) \quad \text{is finite} , \tag{E-2b}$$

and

$$C(a - bt, t) = 0 \quad \text{for} \quad 0 < t < a/b . \tag{E-2c}$$

For this problem the initial condition, (E-2a), shall be assumed to be a constant, C_0; here,

$$C(r, 0) = C_0 \quad \text{for} \quad 0 < r < a . \tag{E-3}$$

If this substitution and $S(r, t; \xi + 2na)$ are made into Eq. (E-1), then

$$C(r,t) = \frac{C_0}{2r(\pi D t)^{1/2}} \left(\int_{-a}^{a} \xi \exp\left[-\frac{(r-\xi)^2}{4Dt}\right] d\xi \right.$$

$$+ \sum_{n=1}^{\infty} \int_{-a}^{a} \xi \exp\left[\frac{nb}{D}(\xi+na)\right] \left\{ \exp\left\{-\frac{[r-(\xi+2na)]^2}{4Dt}\right\} \right. \qquad \text{(E-4)}$$

$$\left. \left. - \exp\left\{-\frac{[r+(\xi+2na)]^2}{4Dt}\right\}\right\} d\xi \right).$$

The first term may be integrated by parts, by letting

$$u = \xi$$

and

$$dv = \exp\left[-\frac{(r-\xi)^2}{4Dt}\right] d\xi;$$

if the second term is rewritten, then

$$C(r,t) = \frac{C_0 a}{2r}\left[\operatorname{erfc}\frac{r-a}{2(Dt)^{1/2}} + \operatorname{erfc}\frac{r+a}{2(Dt)^{1/2}}\right] - \frac{C_0}{2r}\int_{-a}^{a}\operatorname{erfc}\frac{r-\xi}{2(Dt)^{1/2}}\, d\xi$$

$$+ \frac{C_0}{2r(\pi Dt)^{1/2}}\sum_{n=1}^{\infty} \exp\left[\frac{nb}{D}(na)\right]\int_{-a}^{a}\xi\exp\left(\frac{nb\xi}{D}\right)\left(\exp\left\{-\frac{[r-(\xi+2na)]^2}{4Dt}\right\}\right. \qquad \text{(E-5)}$$

$$\left. - \exp\left\{-\frac{[r+(\xi+2na)]^2}{4Dt}\right\}\right) d\xi.$$

The exponentials may be simplified, as follows:

$$\frac{[r-(\xi+2na)]^2}{4Dt} - \frac{nb\xi}{D} = \frac{1}{4Dt}\left[r^2 - 2r(\xi+2na) + (\xi+2na)^2 - 4nbt\xi\right]$$

$$= \frac{1}{4Dt}\left[\xi^2 + 4na\xi - 4nbt\xi - 2r\xi - 4nar + 4n^2a^2 + r^2\right]$$

$$= \frac{1}{4Dt}\left[\xi^2 - 2\xi(r-2na+2nbt) - 4nar + 4n^2a^2 + r^2\right]$$

$$= \frac{1}{4Dt}\Big[(r-2na+2nbt)^2 - 2\xi(r-2na+2nbt) + \xi^2 \\ + r^2 - (r-2na+2nbt)^2 - 4nar + 4n^2a^2\Big] \tag{E-6a}$$

$$= \frac{1}{4Dt}\left[(r-2na+2nbt)-\xi\right]^2 - \frac{1}{4Dt}\Big[r^2 - 4nr(a-bt) + 4n^2(a-bt)^2 \\ + 4nar - 4n^2a^2 - r^2\Big]$$

$$= \frac{1}{4Dt}\left[(r-2na+2nbt)-\xi\right]^2 - \frac{1}{4Dt}\Big[-4nar + 4nbtr + 4n^2a^2 \\ - 8n^2abt + 4nbt(nbt) + 4nar - 4n^2a^2\Big]$$

$$= \frac{1}{4Dt}\left[(r-2na+2nbt)-\xi\right]^2 - \frac{nb}{D}\left[r - 2na + nbt\right],$$

and $\dfrac{[r+(\xi+2na)]^2}{4Dt} - \dfrac{nb\xi}{D} = \dfrac{1}{4Dt}\left[r^2 + 2r(\xi+2na) + (\xi+2na)^2 - 4nbt\xi\right]$

$$= \frac{1}{4Dt}\left[\xi^2 + 4na\xi - 4nbt\xi + 2r\xi + 4nar + 4n^2a^2 + r^2\right]$$

$$= \frac{1}{4Dt}\left[\xi^2 + 2\xi(r+2na-2nbt) + 4nar + 4n^2a^2 + r^2\right]$$

$$= \frac{1}{4Dt}\Big[\xi^2 + 2\xi(r+2na-2nbt) + (r+2na-2nbt)^2 \\ - (r+2na-2nbt)^2 + 4nar + 4n^2a^2 + r^2\Big] \tag{E-6b}$$

$$= \frac{1}{4Dt}\left[\xi + (r+2na-2nbt)\right]^2 - \frac{1}{4Dt}\Big[r^2 + 4nr(a-bt) + 4n^2(a-bt)^2 \\ - 4nar - 4n^2a^2 - r^2\Big]$$

$$= \frac{1}{4Dt}\left[\xi + (r+2na-2nbt)\right]^2 - \frac{1}{4Dt}\Big[4nar - 4nbtr + 4n^2a^2 \\ - 8n^2abt + 4nbt(nbt) - 4nar - 4n^2a^2\Big]$$

$$= \frac{1}{4Dt}\left[\xi + (r+2na-2nbt)\right]^2 - \frac{nb}{D}\left[-r - 2na + nbt\right].$$

Integrating the second term of Eq. (E-5) with the aid of Eq. (C-11), and also substituting the results of Eqs. (E-6a) and (E-6b), one finds

$$\begin{aligned} C(r,t) = {} & \frac{C_0 a}{2r}\left[\operatorname{erfc}\frac{r-a}{2(Dt)^{1/2}} + \operatorname{erfc}\frac{a+r}{2(Dt)^{1/2}}\right] \\ & - \frac{C_0 (Dt)^{1/2}}{r}\left[\operatorname{ierfc}\frac{r-a}{2(Dt)^{1/2}} - \operatorname{ierfc}\frac{a+r}{2(Dt)^{1/2}}\right] \\ & + \frac{C_0}{2r(\pi Dt)^{1/2}}\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt-r)\right]\int_{-a}^{a}\xi\exp\left\{-\frac{[(r-2na+2nbt)-\xi]^2}{4Dt}\right\}d\xi \qquad \text{(E-7)} \\ & - \frac{C_0}{2r(\pi Dt)^{1/2}}\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt+r)\right]\int_{-a}^{a}\xi\exp\left\{-\frac{[(r+2na-2nbt)+\xi]^2}{4Dt}\right\}d\xi . \end{aligned}$$

The remaining integrals may be solved as before by integrating by parts. Let

$$u = \xi$$

and let $\quad dv = \exp\left[-\dfrac{(r-2na+2nbt-\xi)^2}{4Dt}\right]d\xi$

and $\quad dv = \exp\left[-\dfrac{(r+2na-2nbt+\xi)^2}{4Dt}\right]d\xi ,\quad$ successively; then

$$\begin{aligned} C(r,t) = {} & \frac{C_0 a}{2r}\left[\operatorname{erfc}\frac{r-a}{2(Dt)^{1/2}} + \operatorname{erfc}\frac{a+r}{2(Dt)^{1/2}}\right] \\ & - \frac{C_0 (Dt)^{1/2}}{r}\left[\operatorname{ierfc}\frac{r-a}{2(Dt)^{1/2}} - \operatorname{ierfc}\frac{a+r}{2(Dt)^{1/2}}\right] \\ & + \frac{C_0 a}{2r}\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt-r)\right]\left[\operatorname{erfc}\frac{r-2na+2nbt-a}{2(Dt)^{1/2}}\right. \\ & \qquad \left. + \operatorname{erfc}\frac{r-2na+2nbt+a}{2(Dt)^{1/2}}\right] \\ & + \frac{C_0 a}{2r}\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt+r)\right]\left[\operatorname{erfc}\frac{r+2na-2nbt+a}{2(Dt)^{1/2}} + \operatorname{erfc}\frac{r+2na-2nbt-a}{2(Dt)^{1/2}}\right] - \end{aligned}$$

$$
\begin{aligned}
&-\frac{C_0}{2r}\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt-r)\right]\int_{-a}^{a}\operatorname{erfc}\frac{r-2na+2nbt-\xi}{2(Dt)^{1/2}}\,d\xi \\
&-\frac{C_0}{2r}\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt+r)\right]\int_{-a}^{a}\operatorname{erfc}\frac{r+2na-2nbt+\xi}{2(Dt)^{1/2}}\,d\xi .
\end{aligned}
\tag{E-8}
$$

Upon integration of the last two terms of (E-8), one has

$$
\begin{aligned}
C(r,t)=\ &\frac{C_0 a}{2r}\left[\operatorname{erfc}\frac{r-a}{2(Dt)^{1/2}}+\operatorname{erfc}\frac{a+r}{2(Dt)^{1/2}}\right] \\
&-\frac{C_0(Dt)^{1/2}}{r}\left[\operatorname{ierfc}\frac{r-a}{2(Dt)^{1/2}}-\operatorname{ierfc}\frac{a+r}{2(Dt)^{1/2}}\right] \\
&+\frac{C_0 a}{2r}\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt-r)\right]\left[\operatorname{erfc}\frac{r-2na+2nbt-a}{2(Dt)^{1/2}}\right. \\
&\qquad\qquad\left.+\operatorname{erfc}\frac{r-2na+2nbt+a}{2(Dt)^{1/2}}\right] \\
&+\frac{C_0 a}{2r}\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt+r)\right]\left[\operatorname{erfc}\frac{r+2na-2nbt+a}{2(Dt)^{1/2}}\right. \\
&\qquad\qquad\left.+\operatorname{erfc}\frac{r+2na-2nbt-a}{2(Dt)^{1/2}}\right] \\
&-\frac{C_0(Dt)^{1/2}}{r}\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt-r)\right]\left[\operatorname{ierfc}\frac{r-2na+2nbt-a}{2(Dt)^{1/2}}\right. \\
&\qquad\qquad\left.-\operatorname{ierfc}\frac{r-2na+2nbt+a}{2(Dt)^{1/2}}\right] \\
&+\frac{C_0(Dt)^{1/2}}{r}\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt+r)\right]\left[\operatorname{ierfc}\frac{r+2na-2nbt+a}{2(Dt)^{1/2}}\right. \\
&\qquad\qquad\left.-\operatorname{ierfc}\frac{r+2na-2nbt-a}{2(Dt)^{1/2}}\right].
\end{aligned}
\tag{E-9}
$$

By using Eq. (C-12), one obtains

$$
\begin{aligned}
&\operatorname{erfc}\frac{r-2na+2nbt-a}{2(Dt)^{1/2}}+\operatorname{erfc}\frac{r-2na+2nbt+a}{2(Dt)^{1/2}} \\
&=2-\operatorname{erfc}\frac{2na-2nbt+a-r}{2(Dt)^{1/2}}+2-\operatorname{erfc}\frac{2na-2nbt-r-a}{2(Dt)^{1/2}}
\end{aligned}
\tag{E-10a}
$$

and

$$
\operatorname{erfc}\frac{r-a}{2(Dt)^{1/2}}=2-\operatorname{erfc}\frac{a-r}{2(Dt)^{1/2}}. \tag{E-10b}
$$

Using Eq. (C-13), one has

$$\begin{aligned}
&\operatorname{ierfc}\frac{r-2na+2nbt-a}{2(Dt)^{1/2}}-\operatorname{ierfc}\frac{r-2na+2nbt+a}{2(Dt)^{1/2}}\\
&=2\left[\frac{2na-2nbt-r+a}{2(Dt)^{1/2}}\right]+\operatorname{ierfc}\frac{2na-2nbt+a-r}{2(Dt)^{1/2}}\\
&\qquad-2\left[\frac{2na-2nbt-a-r}{2(Dt)^{1/2}}\right]-\operatorname{ierfc}\frac{2na-2nbt-a-r}{2(Dt)^{1/2}}\\
&=\frac{2a}{(Dt)^{1/2}}+\operatorname{ierfc}\frac{2na-2nbt+a-r}{2(Dt)^{1/2}}-\operatorname{ierfc}\frac{2na-2nbt-a-r}{2(Dt)^{1/2}}
\end{aligned}\tag{E-11a}$$

and
$$\operatorname{ierfc}\frac{r-a}{2(Dt)^{1/2}}=2\left[\frac{a-r}{2(Dt)^{1/2}}\right]+\operatorname{ierfc}\frac{a-r}{2(Dt)^{1/2}}.\tag{E-11b}$$

The substitution of Eqs. (E-10) and (E-11) give

$$\begin{aligned}
C(r,t)=&(2)\left(\frac{C_0a}{2r}\right)+\frac{C_0a}{2r}\left[\operatorname{erfc}\frac{a+r}{2(Dt)^{1/2}}-\operatorname{erfc}\frac{a-r}{2(Dt)^{1/2}}\right]\\
&-\left[\frac{C_0(Dt)^{1/2}}{r}\right]\left[\frac{a-r}{2(Dt)^{1/2}}\right]-\frac{C_0(Dt)^{1/2}}{r}\left[\operatorname{ierfc}\frac{a-r}{2(Dt)^{1/2}}-\operatorname{ierfc}\frac{a+r}{2(Dt)^{1/2}}\right]\\
&+(4)\left(\frac{C_0a}{2r}\right)\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt-r)\right]\\
&-\frac{C_0a}{2r}\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt-r)\right]\left[\operatorname{erfc}\frac{2na-2nbt+a-r}{2(Dt)^{1/2}}\right.\\
&\qquad\left.+\operatorname{erfc}\frac{2na-2nbt-a-r}{2(Dt)^{1/2}}\right]\\
&+\frac{C_0a}{2r}\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt+r)\right]\left[\operatorname{erfc}\frac{2na-2nbt+a+r}{2(Dt)^{1/2}}\right.\\
&\qquad\left.+\operatorname{erfc}\frac{2na-2nbt-a+r}{2(Dt)^{1/2}}\right]\\
&-\left[\frac{C_0(Dt)^{1/2}}{r}\right]\left[\frac{2a}{(Dt)^{1/2}}\right]\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt-r)\right]-
\end{aligned}$$

$$- \frac{C_0 (Dt)^{1/2}}{r} \sum_{n=1}^{\infty} \exp\left[-\frac{nb}{D}(na-nbt-r)\right]\left[\operatorname{ierfc}\frac{2na-2nbt+a-r}{2(Dt)^{1/2}} - \operatorname{ierfc}\frac{2na-2nbt-a-r}{2(Dt)^{1/2}}\right] \tag{E-12}$$

$$+ \frac{C_0 (Dt)^{1/2}}{r} \sum_{n=1}^{\infty} \exp\left[-\frac{nb}{D}(na-nbt+r)\right]\left[\operatorname{ierfc}\frac{2na-2nbt+a+r}{2(Dt)^{1/2}} - \operatorname{ierfc}\frac{2na-2nbt-a+r}{2(Dt)^{1/2}}\right].$$

Upon cancelation and rearrangement, one has

$$\begin{aligned}
C(r,t) = {} & C_0 - \frac{C_0 a}{2r}\left[\operatorname{erfc}\frac{a-r}{2(Dt)^{1/2}} - \operatorname{erfc}\frac{a+r}{2(Dt)^{1/2}}\right] \\
& - \frac{C_0 a}{2r}\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt-r)\right]\left[\operatorname{erfc}\frac{2n(a-bt)+a-r}{2(Dt)^{1/2}} + \operatorname{erfc}\frac{2n(a-bt)-a-r}{2(Dt)^{1/2}}\right] \\
& + \frac{C_0 a}{2r}\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt+r)\right]\left[\operatorname{erfc}\frac{2n(a-bt)+a+r}{2(Dt)^{1/2}} + \operatorname{erfc}\frac{2n(a-bt)-a+r}{2(Dt)^{1/2}}\right] \\
& - \frac{C_0 a}{r}\left(\frac{Dt}{a^2}\right)^{1/2}\left[\operatorname{ierfc}\frac{a-r}{2(Dt)^{1/2}} - \operatorname{ierfc}\frac{a+r}{2(Dt)^{1/2}}\right] \\
& - \frac{C_0 a}{r}\left(\frac{Dt}{a^2}\right)^{1/2}\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt-r)\right]\left[\operatorname{ierfc}\frac{2n(a-bt)+a-r}{2(Dt)^{1/2}} - \operatorname{ierfc}\frac{2n(a-bt)-a-r}{2(Dt)^{1/2}}\right] \\
& + \frac{C_0 a}{r}\left(\frac{Dt}{a^2}\right)^{1/2}\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt+r)\right]\left[\operatorname{ierfc}\frac{2n(a-bt)+a+r}{2(Dt)^{1/2}} - \operatorname{ierfc}\frac{2n(a-bt)-a+r}{2(Dt)^{1/2}}\right].
\end{aligned} \tag{E-13}$$

For $t = 0$, since the $\operatorname{erfc} \infty = 0$, Eq. (E-13) becomes $C(r, 0) = C_0$. For $t = a/b$, which corresponds to total evaporation, the tracer concentration becomes zero. (The proof will not be given here.)

If, in Eq. (E-13), $b = 0$, which corresponds to no evaporation, then

$$C(r,t) = C_0 - \frac{C_0 a}{2r}\left[\operatorname{erfc}\frac{a-r}{2(Dt)^{1/2}} - \operatorname{erfc}\frac{a+r}{2(Dt)^{1/2}}\right] -$$

$$\begin{aligned}
&-\frac{C_0 a}{2r}\sum_{n=1}^{\infty}\Big[\mathrm{erfc}\frac{(2n+1)a-r}{2(Dt)^{1/2}}+\mathrm{erfc}\frac{(2n-1)a-r}{2(Dt)^{1/2}}\\
&\qquad\qquad-\mathrm{erfc}\frac{(2n+1)a+r}{2(Dt)^{1/2}}-\mathrm{erfc}\frac{(2n-1)a+r}{2(Dt)^{1/2}}\Big] \qquad \text{(E-14)}\\
&-\frac{C_0 a}{r}\left(\frac{Dt}{a^2}\right)^{1/2}\Big[\mathrm{ierfc}\frac{a-r}{2(Dt)^{1/2}}-\mathrm{ierfc}\frac{a+r}{2(Dt)^{1/2}}\Big]\\
&-\frac{C_0 a}{r}\left(\frac{Dt}{a^2}\right)^{1/2}\sum_{n=1}^{\infty}\Big[\mathrm{ierfc}\frac{(2n+1)a-r}{2(Dt)^{1/2}}-\mathrm{ierfc}\frac{(2n-1)a-r}{2(Dt)^{1/2}}\\
&\qquad\qquad-\mathrm{ierfc}\frac{(2n+1)a+r}{2(Dt)^{1/2}}+\mathrm{ierfc}\frac{(2n-1)a+r}{2(Dt)^{1/2}}\Big].
\end{aligned}$$

If $2n-1=2m+1$, Eq. (E-14) becomes

$$\begin{aligned}
C(r,t) &= C_0-\frac{C_0 a}{2r}\Big[\mathrm{erfc}\frac{a-r}{2(Dt)^{1/2}}-\mathrm{erfc}\frac{a+r}{2(Dt)^{1/2}}\Big]\\
&\quad-\frac{C_0 a}{2r}\sum_{n=1}^{\infty}\Big[\mathrm{erfc}\frac{(2n+1)a-r}{2(Dt)^{1/2}}-\mathrm{erfc}\frac{(2n+1)a+r}{2(Dt)^{1/2}}\Big]\\
&\quad-\frac{C_0 a}{2r}\sum_{m=0}^{\infty}\Big[\mathrm{erfc}\frac{(2m+1)a-r}{2(Dt)^{1/2}}-\mathrm{erfc}\frac{(2m+1)a+r}{2(Dt)^{1/2}}\Big]\\
&\quad-\frac{C_0 a}{r}\left(\frac{Dt}{a^2}\right)^{1/2}\Big[\mathrm{ierfc}\frac{a-r}{2(Dt)^{1/2}}-\mathrm{ierfc}\frac{a+r}{2(Dt)^{1/2}}\Big]\\
&\quad-\frac{C_0 a}{r}\left(\frac{Dt}{a^2}\right)^{1/2}\sum_{n=1}^{\infty}\Big[\mathrm{ierfc}\frac{(2n+1)a-r}{2(Dt)^{1/2}}-\mathrm{ierfc}\frac{(2n+1)a+r}{2(Dt)^{1/2}}\Big]\\
&\quad+\frac{C_0 a}{r}\left(\frac{Dt}{a^2}\right)^{1/2}\sum_{m=0}^{\infty}\Big[\mathrm{ierfc}\frac{(2m+1)a-r}{2(Dt)^{1/2}}-\mathrm{ierfc}\frac{(2m+1)a+r}{2(Dt)^{1/2}}\Big]\\
&= C_0-\frac{C_0 a}{2r}\sum_{n=0}^{\infty}\Big[\mathrm{erfc}\frac{(2n+1)a-r}{2(Dt)^{1/2}}-\mathrm{erfc}\frac{(2n+1)a+r}{2(Dt)^{1/2}}\Big]\\
&\quad-\frac{C_0 a}{2r}\sum_{m=0}^{\infty}\Big[\mathrm{erfc}\frac{(2m+1)a-r}{2(Dt)^{1/2}}-\mathrm{erfc}\frac{(2m+1)a+r}{2(Dt)^{1/2}}\Big]\\
&\quad-\frac{C_0 a}{r}\left(\frac{Dt}{a^2}\right)^{1/2}\sum_{n=0}^{\infty}\Big[\mathrm{ierfc}\frac{(2n+1)a-r}{2(Dt)^{1/2}}-\mathrm{ierfc}\frac{(2n+1)a+r}{2(Dt)^{1/2}}\Big]
\end{aligned}$$

$$+\frac{C_0 a}{r}\left(\frac{Dt}{a^2}\right)^{1/2}\sum_{m=0}^{\infty}\left[\text{ierfc}\,\frac{(2m+1)a-r}{2(Dt)^{1/2}}-\text{ierfc}\,\frac{(2m+1)a+r}{2(Dt)^{1/2}}\right] \qquad \text{(E-15)}$$

$$=C_0-\frac{C_0 a}{r}\sum_{n=0}^{\infty}\left[\text{erfc}\,\frac{(2n+1)a-r}{2(Dt)^{1/2}}-\text{erfc}\,\frac{(2n+1)a+r}{2(Dt)^{1/2}}\right],$$

which may be recognized as Eq. (B-6).

E.2. Fractional Release of the Tracer

The fractional release may be computed from Eq. (A-17),

$$f=\frac{Q_0-Q(t)}{Q_0}, \qquad \text{(A-17)}$$

where $Q(t)$ is the total number of tracer atoms contained in the solid at any time t, and $Q_0=\frac{4}{3}\pi a^3 C_0$ is the total number of tracer atoms contained in the solid at time $t=0$.

Thus, $$f=\frac{4/3\,\pi a^3 C_0-\int_0^{(a-bt)}4\pi r^2 C(r,t)\,dr}{4/3\,\pi a^3 C_0}=1-\frac{3}{a^3 C_0}\int_0^{(a-bt)}r^2 C(r,t)\,dr. \qquad \text{(E-16)}$$

With the substitution of Eq. (E-13) into Eq. (E-16), one finds

$$f=1-\frac{3}{a^3C_0}\int_0^{(a-bt)}r^2C_0\,dr+\frac{3}{a^3C_0}\int_0^{(a-bt)}r^2\left(\frac{C_0a}{2r}\right)\left[\text{erfc}\,\frac{a-r}{2(Dt)^{1/2}}-\text{erfc}\,\frac{a+r}{2(Dt)^{1/2}}\right]dr$$

$$+\frac{3}{a^3C_0}\int_0^{(a-bt)}r^2\left(\frac{C_0a}{2r}\right)\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt-r)\right]\left[\text{erfc}\,\frac{2n(a-bt)+a-r}{2(Dt)^{1/2}}\right.$$

$$\left.+\text{erfc}\,\frac{2n(a-bt)-a-r}{2(Dt)^{1/2}}\right]dr$$

$$-\frac{3}{a^3C_0}\int_0^{(a-bt)}r^2\left(\frac{C_0a}{2r}\right)\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt+r)\right]\left[\text{erfc}\,\frac{2n(a-bt)+a+r}{2(Dt)^{1/2}}\right.$$

$$\left.+\text{erfc}\,\frac{2n(a-bt)-a+r}{2(Dt)^{1/2}}\right]dr\;+$$

$$
\begin{aligned}
&+\frac{3}{a^3C_0}\int_0^{(a-bt)} r^2\left(\frac{C_0a}{r}\right)\left(\frac{Dt}{a^2}\right)^{1/2}\left[i\,\mathrm{erfc}\,\frac{a-r}{2(Dt)^{1/2}} - i\,\mathrm{erfc}\,\frac{a+r}{2(Dt)^{1/2}}\right]dr \\
&+\frac{3}{a^3C_0}\int_0^{(a-bt)} r^2\left(\frac{C_0a}{r}\right)\left(\frac{Dt}{a^2}\right)^{1/2}\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt-r)\right]\left[i\,\mathrm{erfc}\,\frac{2n(a-bt)+a-r}{2(Dt)^{1/2}}\right. \\
&\qquad\qquad\left. - i\,\mathrm{erfc}\,\frac{2n(a-bt)-a-r}{2(Dt)^{1/2}}\right]dr \\
&-\frac{3}{a^3C_0}\int_0^{(a-bt)} r^2\left(\frac{C_0a}{r}\right)\left(\frac{Dt}{a^2}\right)^{1/2}\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt+r)\right]\left[i\,\mathrm{erfc}\,\frac{2n(a-bt)+a+r}{2(Dt)^{1/2}}\right. \\
&\qquad\qquad\left. - i\,\mathrm{erfc}\,\frac{2n(a-bt)-a+r}{2(Dt)^{1/2}}\right]dr \\
&= 1-\frac{3}{a^3}\int_0^{(a-bt)} r^2\,dr + \frac{3}{2a^2}\int_0^{(a-bt)} r\left[\mathrm{erfc}\,\frac{a-r}{2(Dt)^{1/2}} - \mathrm{erfc}\,\frac{a+r}{2(Dt)^{1/2}}\right]dr \\
&+\frac{3}{2a^2}\int_0^{(a-bt)} r\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt-r)\right]\left[\mathrm{erfc}\,\frac{2n(a-bt)+a-r}{2(Dt)^{1/2}}\right. \\
&\qquad\qquad\left. + \mathrm{erfc}\,\frac{2n(a-bt)-a-r}{2(Dt)^{1/2}}\right]dr \\
&-\frac{3}{2a^2}\int_0^{(a-bt)} r\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt+r)\right]\left[\mathrm{erfc}\,\frac{2n(a-bt)+a+r}{2(Dt)^{1/2}}\right. \\
&\qquad\qquad\left. + \mathrm{erfc}\,\frac{2n(a-bt)-a+r}{2(Dt)^{1/2}}\right]dr \\
&+\frac{3}{a^2}\left(\frac{Dt}{a^2}\right)^{1/2}\int_0^{(a-bt)} r\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt-r)\right]\left[i\,\mathrm{erfc}\,\frac{2n(a-bt)+a-r}{2(Dt)^{1/2}}\right. \\
&\qquad\qquad\left. - i\,\mathrm{erfc}\,\frac{2n(a-bt)-a-r}{2(Dt)^{1/2}}\right]dr \\
&-\frac{3}{a^2}\left(\frac{Dt}{a^2}\right)^{1/2}\int_0^{(a-bt)} r\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt+r)\right]\left[i\,\mathrm{erfc}\,\frac{2n(a-bt)+a+r}{2(Dt)^{1/2}}\right. \\
&\qquad\qquad\left. - i\,\mathrm{erfc}\,\frac{2n(a-bt)-a+r}{2(Dt)^{1/2}}\right]dr \\
&+\frac{3}{a^2}\left(\frac{Dt}{a^2}\right)^{1/2}\int_0^{(a-bt)} r\left[i\,\mathrm{erfc}\,\frac{a-r}{2(Dt)^{1/2}} - i\,\mathrm{erfc}\,\frac{a+r}{2(Dt)^{1/2}}\right]dr .
\end{aligned}
\tag{E-17}
$$

The first integral in Eq. (E-17) may be handled directly, whereas the second and last integrals may be handled by integrating by parts twice, as follows with the use of Eq. (C-11)

$$u = r, \qquad dv_1 = i^n\mathrm{erfc}\,\frac{a-r}{2(Dt)^{1/2}}\,dr, \quad \text{where } n = 0, 1,$$

$$du = dr, \text{ and } \quad v_1 = 2(Dt)^{1/2}\, i^{n+1}\mathrm{erfc}\,\frac{a-r}{2(Dt)^{1/2}},$$

or $dv_2 = i^n\operatorname{erfc}\frac{a+r}{2(Dt)^{1/2}}dr$, and $v_2 = -2(Dt)^{1/2}i^{n+1}\operatorname{erfc}\frac{a+r}{2(Dt)^{1/2}}$.

Hence,

$$\begin{aligned}
f = {} & 1 - \frac{1}{a^3}(a-bt)^3 + \frac{3}{2a^2}\left[2(Dt)^{1/2}\right]\Big[(a-bt)\,i\operatorname{erfc}\frac{bt}{2(Dt)^{1/2}} \\
& \qquad + (a-bt)\,i\operatorname{erfc}\frac{2a-bt}{2(Dt)^{1/2}}\Big] \\
& + \frac{3}{2a^2}\left[2(Dt)^{1/2}\right]\left[-2(Dt)^{1/2}i^2\operatorname{erfc}\frac{bt}{2(Dt)^{1/2}} + 2(Dt)^{1/2}i^2\operatorname{erfc}\frac{2a-bt}{2(Dt)^{1/2}}\right] \\
& + \frac{3}{a^2}\left(\frac{Dt}{a^2}\right)^{1/2}\left[2(Dt)^{1/2}\right]\left[(a-bt)\,i^2\operatorname{erfc}\frac{bt}{2(Dt)^{1/2}} + (a-bt)\,i^2\operatorname{erfc}\frac{2a-bt}{2(Dt)^{1/2}}\right] \\
& + \frac{3}{a^2}\left(\frac{Dt}{a^2}\right)^{1/2}\left[2(Dt)^{1/2}\right]\left[-2(Dt)^{1/2}i^3\operatorname{erfc}\frac{bt}{2(Dt)^{1/2}} + 2(Dt)^{1/2}i^3\operatorname{erfc}\frac{2a-bt}{2(Dt)^{1/2}}\right] \\
& + \frac{3}{2a^2}\int_0^{(a-bt)} r\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt-r)\right]\Big[\operatorname{erfc}\frac{2n(a-bt)+a-r}{2(Dt)^{1/2}} \\
& \qquad + \operatorname{erfc}\frac{2n(a-bt)-a-r}{2(Dt)^{1/2}}\Big]dr \\
& - \frac{3}{2a^2}\int_0^{(a-bt)} r\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt+r)\right]\Big[\operatorname{erfc}\frac{2n(a-bt)+a+r}{2(Dt)^{1/2}} \\
& \qquad + \operatorname{erfc}\frac{2n(a-bt)-a+r}{2(Dt)^{1/2}}\Big]dr \\
& + \frac{3}{a^2}\left(\frac{Dt}{a^2}\right)^{1/2}\int_0^{(a-bt)} r\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt-r)\right]\Big[i\operatorname{erfc}\frac{2n(a-bt)+a-r}{2(Dt)^{1/2}} \\
& \qquad - i\operatorname{erfc}\frac{2n(a-bt)-a-r}{2(Dt)^{1/2}}\Big]dr \\
& - \frac{3}{a^2}\left(\frac{Dt}{a^2}\right)^{1/2}\int_0^{(a-bt)} r\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt+r)\right]\Big[i\operatorname{erfc}\frac{2n(a-bt)+a+r}{2(Dt)^{1/2}} \\
& \qquad - i\operatorname{erfc}\frac{2n(a-bt)-a+r}{2(Dt)^{1/2}}\Big]dr \\
= {} & 3\left(\frac{bt}{a}\right) - 3\left(\frac{bt}{a}\right)^2 + \left(\frac{bt}{a}\right)^3 \\
& + 3\left(\frac{Dt}{a^2}\right)^{1/2}\left(\frac{a-bt}{a}\right)\left[i\operatorname{erfc}\frac{bt}{2(Dt)^{1/2}} + i\operatorname{erfc}\frac{2a-bt}{2(Dt)^{1/2}}\right] \\
& - 6\left(\frac{Dt}{a^2}\right)\left[i^2\operatorname{erfc}\frac{bt}{2(Dt)^{1/2}} - i^2\operatorname{erfc}\frac{2a-bt}{2(Dt)^{1/2}}\right] +
\end{aligned}$$

$$
\begin{aligned}
&+6\left(\frac{Dt}{a^2}\right)\left(\frac{a-bt}{a}\right)\left[i^2\operatorname{erfc}\frac{bt}{2(Dt)^{1/2}}+i^2\operatorname{erfc}\frac{2a-bt}{2(Dt)^{1/2}}\right]\\
&-12\left(\frac{Dt}{a^2}\right)^{3/2}\left[i^3\operatorname{erfc}\frac{bt}{2(Dt)^{1/2}}-i^3\operatorname{erfc}\frac{2a-bt}{2(Dt)^{1/2}}\right]\\
&+\frac{3}{2a^2}\int_0^{(a-bt)} r\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt-r)\right]\left[\operatorname{erfc}\frac{2n(a-bt)+a-r}{2(Dt)^{1/2}}\right.\\
&\qquad\qquad\left.+\operatorname{erfc}\frac{2n(a-bt)-a-r}{2(Dt)^{1/2}}\right]dr\\
&-\frac{3}{2a^2}\int_0^{(a-bt)} r\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt+r)\right]\left[\operatorname{erfc}\frac{2n(a-bt)+a+r}{2(Dt)^{1/2}}\right.\\
&\qquad\qquad\left.+\operatorname{erfc}\frac{2n(a-bt)-a+r}{2(Dt)^{1/2}}\right]dr\\
&+\frac{3}{a^2}\left(\frac{Dt}{a^2}\right)^{1/2}\int_0^{(a-bt)} r\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt-r)\right]\left[i\operatorname{erfc}\frac{2n(a-bt)+a-r}{2(Dt)^{1/2}}\right.\\
&\qquad\qquad\left.-i\operatorname{erfc}\frac{2n(a-bt)-a-r}{2(Dt)^{1/2}}\right]dr\\
&-\frac{3}{a^2}\left(\frac{Dt}{a^2}\right)^{1/2}\int_0^{(a-bt)} r\sum_{n=1}^{\infty}\exp\left[-\frac{nb}{D}(na-nbt+r)\right]\left[i\operatorname{erfc}\frac{2n(a-bt)+a+r}{2(Dt)^{1/2}}\right.\\
&\qquad\qquad\left.-i\operatorname{erfc}\frac{2n(a-bt)-a+r}{2(Dt)^{1/2}}\right]dr.
\end{aligned}
\tag{E-18}
$$

The remaining integrals in the expression (E-18) for the fractional release may be evaluated by integrating by parts, as follows:

$$u = r\exp\left[-\frac{nb}{D}(na-nbt-r)\right],$$

$$du = r\left(\frac{nb}{D}\right)\exp\left[-\frac{nb}{D}(na-nbt-r)\right]dr+\exp\left[-\frac{nb}{D}(na-nbt-r)\right]dr,$$

$$dv = \operatorname{erfc}\frac{2n(a-bt)\pm a-r}{2(Dt)^{1/2}}\,dr,$$

and $$V = 2(Dt)^{1/2}\,i\operatorname{erfc}\frac{2n(a-bt)\pm a-r}{2(Dt)^{1/2}}.$$

Several repetitions may be required before the pattern that develops becomes obvious. The result is

$$2(Dt)^{1/2}(a-bt)\exp\left[-\frac{nb}{D}(na-nbt-r)\right]\sum_{m=1}^{\infty}(-1)^{m+1}\left[2\left(\frac{nb}{D}\right)(Dt)^{1/2}\right]^{m-1} i^m\mathrm{erfc}\,\frac{2n(a-bt)\pm a-r}{2(Dt)^{1/2}}$$

(E-19)

$$+4(Dt)\exp\left[-\frac{nb}{D}(na-nbt-r)\right]\sum_{m=2}^{\infty}(-1)^{m+1}(m-1)\left[2\left(\frac{nb}{D}\right)(Dt)^{1/2}\right]^{m-2} i^m\mathrm{erfc}\,\frac{2n(a-bt)\pm a-r}{2(Dt)^{1/2}}\ .$$

The similar integral, which would have $dv = \mathrm{ierfc}\,\frac{2n(a-bt)\pm a-r}{2\sqrt{Dt}}\,dr$, differs from Eq. (E-19) only in the power of the ierfc x term. If m were replaced by m + 1, the result [Eq. (E-19)] could be used as it is.

The remaining form of the integral to be evaluated by parts is

$$u = r\exp\left[-\frac{nb}{D}(na-nbt+r)\right],$$

$$du = -r\left(\frac{nb}{D}\right)\exp\left[-\frac{nb}{D}(na-nbt+r)\right]dr + \exp\left[-\frac{nb}{D}(na-nbt+r)\right]dr,$$

$$dv = \mathrm{erfc}\,\frac{2n(a-bt)\pm a+r}{2(Dt)^{1/2}}\,dr\ ,$$

and $$V = -2(Dt)^{1/2}\,\mathrm{ierfc}\,\frac{2n(a-bt)\pm a+r}{2(Dt)^{1/2}}\ .$$

After several repetitions the result may be recognized as

$$-2(Dt)^{1/2}(a-bt)\exp\left[-\frac{nb}{D}(na-nbt+r)\right]\sum_{m=1}^{\infty}(-1)^{m+1}\left[2\left(\frac{nb}{D}\right)(Dt)^{1/2}\right]^{m-1} i^m\mathrm{erfc}\,\frac{2n(a-bt)\pm a+r}{2(Dt)^{1/2}}$$

(E-20)

$$+4(Dt)\exp\left[-\frac{nb}{D}(na-nbt+r)\right]\sum_{m=2}^{\infty}(-1)^{m+1}(m-1)\left[2\left(\frac{nb}{D}\right)(Dt)^{1/2}\right]^{m-2} i^m\mathrm{erfc}\,\frac{2n(a-bt)\pm a+r}{2(Dt)^{1/2}}.$$

Upon applying limits to Eqs. (E-19) and (E-20), the resulting terms are inserted into Eq. (E-18) to give

$$
\begin{aligned}
f = {} & 3\left(\frac{bt}{a}\right) - 3\left(\frac{bt}{a}\right)^2 + \left(\frac{bt}{a}\right)^3 + 3\left(\frac{Dt}{a^2}\right)^{1/2}\left(\frac{a-bt}{a}\right)\left[i\mathrm{erfc}\,\frac{bt}{2(Dt)^{1/2}} + i\mathrm{erfc}\,\frac{2a-bt}{2(Dt)^{1/2}}\right] \\
& - 6\left(\frac{Dt}{a^2}\right)\left[i^2\mathrm{erfc}\,\frac{bt}{2(Dt)^{1/2}} - i^2\mathrm{erfc}\,\frac{2a-bt}{2(Dt)^{1/2}}\right] + 6\left(\frac{Dt}{a^2}\right)\left(\frac{a-bt}{a}\right)\left[i^2\mathrm{erfc}\,\frac{bt}{2(Dt)^{1/2}}\right. \\
& \left. + i^2\mathrm{erfc}\,\frac{2a-bt}{2(Dt)^{1/2}}\right] - 12\left(\frac{Dt}{a^2}\right)^{3/2}\left[i^3\mathrm{erfc}\,\frac{bt}{2(Dt)^{1/2}} - i^3\mathrm{erfc}\,\frac{2a-bt}{2(Dt)^{1/2}}\right] \\
& + 3\left(\frac{Dt}{a^2}\right)^{1/2}\left(\frac{a-bt}{a}\right)\sum_{n,m=1}^{\infty}(-1)^{m+1}\left[2\left(\frac{nb}{D}\right)(Dt)^{1/2}\right]^{m-1}\exp\left[-\frac{nb}{D}(n-1)(a-bt)\right]\left[i^m\mathrm{erfc}\,\frac{(2n-1)(a-bt)+a}{2(Dt)^{1/2}}\right. \\
& \qquad \left. + i^m\mathrm{erfc}\,\frac{(2n-1)(a-bt)-a}{2(Dt)^{1/2}}\right] \\
& + 3\left(\frac{Dt}{a^2}\right)^{1/2}\left(\frac{a-bt}{a}\right)\sum_{n,m=1}^{\infty}(-1)^{m+1}\left[2\left(\frac{nb}{D}\right)(Dt)^{1/2}\right]^{m-1}\exp\left[-\frac{nb}{D}(n+1)(a-bt)\right]\left[i^m\mathrm{erfc}\,\frac{(2n+1)(a-bt)+a}{2(Dt)^{1/2}}\right. \\
& \qquad \left. + i^m\mathrm{erfc}\,\frac{(2n+1)(a-bt)-a}{2(Dt)^{1/2}}\right] \\
& + 6\left(\frac{Dt}{a^2}\right)\sum_{\substack{n=1\\m=2}}^{\infty}(-1)^{m+1}(m-1)\left[2\left(\frac{nb}{D}\right)(Dt)^{1/2}\right]^{m-2}\exp\left[-\frac{nb}{D}(n-1)(a-bt)\right]\left[i^m\mathrm{erfc}\,\frac{(2n-1)(a-bt)+a}{2(Dt)^{1/2}}\right. \\
& \qquad \left. + i^m\mathrm{erfc}\,\frac{(2n-1)(a-bt)-a}{2(Dt)^{1/2}}\right] \\
& - 6\left(\frac{Dt}{a^2}\right)\sum_{\substack{n=1\\m=2}}^{\infty}(-1)^{m+1}(m-1)\left[2\left(\frac{nb}{D}\right)(Dt)^{1/2}\right]^{m-2}\exp\left[-\frac{nb}{D}(n+1)(a-bt)\right]\left[i^m\mathrm{erfc}\,\frac{(2n+1)(a-bt)+a}{2(Dt)^{1/2}}\right. \\
& \qquad \left. + i^m\mathrm{erfc}\,\frac{(2n+1)(a-bt)-a}{2(Dt)^{1/2}}\right] \\
& + 6\left(\frac{Dt}{a^2}\right)\left(\frac{a-bt}{a}\right)\sum_{\substack{n=1\\m=2}}^{\infty}(-1)^{m}\left[2\left(\frac{nb}{D}\right)(Dt)^{1/2}\right]^{m-2}\exp\left[-\frac{nb}{D}(n-1)(a-bt)\right]\left[i^m\mathrm{erfc}\,\frac{(2n-1)(a-bt)+a}{2(Dt)^{1/2}}\right. \\
& \qquad \left. - i^m\mathrm{erfc}\,\frac{(2n-1)(a-bt)-a}{2(Dt)^{1/2}}\right] \\
& + 6\left(\frac{Dt}{a^2}\right)\left(\frac{a-bt}{a}\right)\sum_{\substack{n=1\\m=2}}^{\infty}(-1)^{m}\left[2\left(\frac{nb}{D}\right)(Dt)^{1/2}\right]^{m-2}\exp\left[-\frac{nb}{D}(n+1)(a-bt)\right]\left[i^m\mathrm{erfc}\,\frac{(2n+1)(a-bt)+a}{2(Dt)^{1/2}}\right. \\
& \qquad \left. - i^m\mathrm{erfc}\,\frac{(2n+1)(a-bt)-a}{2(Dt)^{1/2}}\right] \\
& + 12\left(\frac{Dt}{a^2}\right)^{3/2}\sum_{\substack{n=1\\m=3}}^{\infty}(-1)^{m}(m-2)\left[2\left(\frac{nb}{D}\right)(Dt)^{1/2}\right]^{m-3}\exp\left[-\frac{nb}{D}(n-1)(a-bt)\right]\left[i^m\mathrm{erfc}\,\frac{(2n-1)(a-bt)+a}{2(Dt)^{1/2}}\right. \\
& \qquad \left. - i^m\mathrm{erfc}\,\frac{(2n-1)(a-bt)-a}{2(Dt)^{1/2}}\right] \\
& - 12\left(\frac{Dt}{a^2}\right)^{3/2}\sum_{\substack{n=1\\m=3}}^{\infty}(-1)^{m}(m-2)\left[2\left(\frac{nb}{D}\right)(Dt)^{1/2}\right]^{m-3}\exp\left[-\frac{nb}{D}(n+1)(a-bt)\right]\left[i^m\mathrm{erfc}\,\frac{(2n+1)(a-bt)+a}{2(Dt)^{1/2}}\right. \\
& \qquad \left. - i^m\mathrm{erfc}\,\frac{(2n+1)(a-bt)-a}{2(Dt)^{1/2}}\right],
\end{aligned}
\tag{E-21}
$$

as the solution in full form for the fractional release of the tracer element from a spherical body.

At t = 0, each term of Eq. (E-21) becomes zero; thus the fractional release is zero. At time t = a/b, which corresponds to complete evaporation of the solid, the fractional release should be 1, as follows:

$$f = 3 - 3 + 1 - 6\left(\frac{D}{ab}\right)\left[i^2\text{erfc}\,\frac{a}{2\left(\frac{Da}{b}\right)^{1/2}} - i^2\text{erfc}\,\frac{2a-a}{2\left(\frac{Da}{b}\right)^{1/2}}\right]$$

$$-12\left(\frac{D}{ab}\right)^{3/2}\left[i^3\text{erfc}\,\frac{a}{2\left(\frac{Da}{b}\right)^{1/2}} - i^3\text{erfc}\,\frac{2a-a}{2\left(\frac{Da}{b}\right)^{1/2}}\right]$$

$$+6\left(\frac{D}{ab}\right)\sum_{\substack{n=1\\m=2}}^{\infty}(-1)^{m+1}(m-1)\left[2\left(\frac{nb}{D}\right)\left(\frac{Da}{b}\right)^{1/2}\right]^{m-2}\left[i^m\text{erfc}\,\frac{a}{2\left(\frac{Da}{b}\right)^{1/2}} + i^m\text{erfc}\,\frac{-a}{2\left(\frac{Da}{b}\right)^{1/2}}\right.$$

$$\left. - i^m\text{erfc}\,\frac{a}{2\left(\frac{Da}{b}\right)^{1/2}} - i^m\text{erfc}\,\frac{-a}{2\left(\frac{Da}{b}\right)^{1/2}}\right] \qquad \text{(E-22)}$$

$$+12\left(\frac{D}{ab}\right)^{3/2}\sum_{\substack{n=1\\m=3}}^{\infty}(-1)^{m}(m-2)\left[2\left(\frac{nb}{D}\right)\left(\frac{Da}{b}\right)^{1/2}\right]^{m-3}\left[i^m\text{erfc}\,\frac{a}{2\left(\frac{Da}{b}\right)^{1/2}}\right.$$

$$\left. - i^m\text{erfc}\,\frac{-a}{2\left(\frac{Da}{b}\right)^{1/2}} - i^m\text{erfc}\,\frac{a}{2\left(\frac{Da}{b}\right)^{1/2}} + i^m\text{erfc}\,\frac{-a}{2\left(\frac{Da}{b}\right)^{1/2}}\right]$$

$$= 3 - 3 + 1 = 1.$$

If, in Eq. (E-21), b is set equal to zero, which corresponds to no evaporation, then

$$f = 3\left(\frac{Dt}{a^2}\right)^{1/2}\left[i\text{erfc}\,0 + i\text{erfc}\,\frac{a}{(Dt)^{1/2}}\right] - 6\left(\frac{Dt}{a^2}\right)\left[i^2\text{erfc}\,0 - i^2\text{erfc}\,\frac{a}{(Dt)^{1/2}}\right]$$

$$+ 6\left(\frac{Dt}{a^2}\right)\left[i^2\text{erfc}\,0 + i^2\text{erfc}\,\frac{a}{(Dt)^{1/2}} - 12\left(\frac{Dt}{a^2}\right)^{3/2}\left[i^3\text{erfc}\,0 - i^3\text{erfc}\,\frac{a}{(Dt)^{1/2}}\right] +$$

$$+3\left(\frac{Dt}{a^2}\right)^{1/2}\sum_{n=1}^{\infty}\left[i\text{erfc}\frac{na}{(Dt)^{1/2}}+i\text{erfc}\frac{(n-1)a}{(Dt)^{1/2}}+i\text{erfc}\frac{(n+1)a}{(Dt)^{1/2}}+i\text{erfc}\frac{na}{(Dt)^{1/2}}\right]$$

$$-6\left(\frac{Dt}{a^2}\right)\sum_{n=1}^{\infty}\left[i^2\text{erfc}\frac{na}{(Dt)^{1/2}}+i^2\text{erfc}\frac{(n-1)a}{(Dt)^{1/2}}-i^2\text{erfc}\frac{(n+1)a}{(Dt)^{1/2}}-i^2\text{erfc}\frac{na}{(Dt)^{1/2}}\right]$$

$$+6\left(\frac{Dt}{a^2}\right)\sum_{n=1}^{\infty}\left[i^2\text{erfc}\frac{na}{(Dt)^{1/2}}-i^2\text{erfc}\frac{(n-1)a}{(Dt)^{1/2}}+i^2\text{erfc}\frac{(n+1)a}{(Dt)^{1/2}}-i^2\text{erfc}\frac{na}{(Dt)^{1/2}}\right]$$

$$+12\left(\frac{Dt}{a^2}\right)^{3/2}\sum_{n=1}^{\infty}\left[i^3\text{erfc}\frac{(n+1)a}{(Dt)^{1/2}}-i^3\text{erfc}\frac{na}{(Dt)^{1/2}}-i^3\text{erfc}\frac{na}{(Dt)^{1/2}}+i^3\text{erfc}\frac{(n-1)a}{(Dt)^{1/2}}\right]$$

$$= 3\left(\frac{Dt}{a^2}\right)^{1/2}\left[i\text{erfc}\ 0+i\text{erfc}\frac{a}{(Dt)^{1/2}}\right] \tag{E-23}$$

$$+6\left(\frac{Dt}{a^2}\right)\left[i^2\text{erfc}\frac{a}{(Dt)^{1/2}}+i^2\text{erfc}\frac{a}{(Dt)^{1/2}}\right]-12\left(\frac{Dt}{a^2}\right)^{3/2}\left[i^3\text{erfc}\ 0-i^3\text{erfc}\frac{a}{(Dt)^{1/2}}\right]$$

$$+3\left(\frac{Dt}{a^2}\right)^{1/2}\sum_{n=1}^{\infty}\left[i\text{erfc}\frac{(n+1)a}{(Dt)^{1/2}}+2\,i\text{erfc}\frac{na}{(Dt)^{1/2}}+i\text{erfc}\frac{(n-1)a}{(Dt)^{1/2}}\right]$$

$$-6\left(\frac{Dt}{a^2}\right)\sum_{n=1}^{\infty}\left[i^2\text{erfc}\frac{(n-1)a}{(Dt)^{1/2}}-i^2\text{erfc}\frac{(n+1)a}{(Dt)^{1/2}}-i^2\text{erfc}\frac{(n+1)a}{(Dt)^{1/2}}+i^2\text{erfc}\frac{(n-1)a}{(Dt)^{1/2}}\right]$$

$$+12\left(\frac{Dt}{a^2}\right)^{3/2}\sum_{n=1}^{\infty}\left[i^3\text{erfc}\frac{(n+1)a}{(Dt)^{1/2}}-2\,i^3\text{erfc}\frac{na}{(Dt)^{1/2}}+i^3\text{erfc}\frac{(n-1)a}{(Dt)^{1/2}}\right].$$

By letting $n + 1 = m$ and $n - 1 = p$, one obtains

$$f = 3\left(\frac{Dt}{a^2}\right)^{1/2}\left[i\text{erfc}\ 0+i\text{erfc}\frac{a}{(Dt)^{1/2}}\right]+12\left(\frac{Dt}{a^2}\right)i^2\text{erfc}\frac{a}{(Dt)^{1/2}}$$

$$-12\left(\frac{Dt}{a^2}\right)^{3/2}\left[i^3\text{erfc}\ 0-i^3\text{erfc}\frac{a}{(Dt)^{1/2}}\right]+$$

$$\begin{aligned}
&+3\left(\frac{Dt}{a^2}\right)^{1/2}\left[\sum_{m=2}^{\infty}\operatorname{ierfc}\frac{ma}{(Dt)^{1/2}}+2\sum_{n=1}^{\infty}\operatorname{ierfc}\frac{na}{(Dt)^{1/2}}+\sum_{p=0}^{\infty}\operatorname{ierfc}\frac{pa}{(Dt)^{1/2}}\right]\\
&-12\left(\frac{Dt}{a^2}\right)\left[\sum_{p=0}^{\infty}i^2\operatorname{erfc}\frac{pa}{(Dt)^{1/2}}-\sum_{m=2}^{\infty}i^2\operatorname{erfc}\frac{ma}{(Dt)^{1/2}}\right]\\
&+12\left(\frac{Dt}{a^2}\right)^{3/2}\left[\sum_{m=2}^{\infty}i^3\operatorname{erfc}\frac{ma}{(Dt)^{1/2}}-2\sum_{n=1}^{\infty}i^3\operatorname{erfc}\frac{na}{(Dt)^{1/2}}+\sum_{p=0}^{\infty}i^3\operatorname{erfc}\frac{pa}{(Dt)^{1/2}}\right]\\
&=3\left(\frac{Dt}{a^2}\right)^{1/2}\left[2\operatorname{ierfc}0+\sum_{m=1}^{\infty}\operatorname{ierfc}\frac{ma}{(Dt)^{1/2}}+2\sum_{n=1}^{\infty}\operatorname{ierfc}\frac{na}{(Dt)^{1/2}}+\sum_{p=1}^{\infty}\operatorname{ierfc}\frac{pa}{(Dt)^{1/2}}\right]\\
&\quad+12\left(\frac{Dt}{a^2}\right)\left[\sum_{m=1}^{\infty}i^2\operatorname{erfc}\frac{ma}{(Dt)^{1/2}}-\sum_{p=1}^{\infty}i^2\operatorname{erfc}\frac{pa}{(Dt)^{1/2}}-i^2\operatorname{erfc}0\right]\\
&\quad+12\left(\frac{Dt}{a^2}\right)^{3/2}\left[\sum_{m=1}^{\infty}i^3\operatorname{erfc}\frac{ma}{(Dt)^{1/2}}-2\sum_{n=1}^{\infty}i^3\operatorname{erfc}\frac{na}{(Dt)^{1/2}}\right.\\
&\qquad\qquad\left.+\sum_{p=1}^{\infty}i^3\operatorname{erfc}\frac{pa}{(Dt)^{1/2}}+i^3\operatorname{erfc}0-i^3\operatorname{erfc}0\right]\\
&=6\left(\frac{Dt}{a^2}\right)^{1/2}\left[\operatorname{ierfc}0+2\sum_{n=1}^{\infty}\operatorname{ierfc}\frac{na}{(Dt)^{1/2}}\right]\\
&\quad-12\left(\frac{Dt}{a^2}\right)i^2\operatorname{erfc}0\,.
\end{aligned}\tag{E-24}$$

Because $\operatorname{ierfc}0=\pi^{-1/2}$ and $i^2\operatorname{erfc}0=1/4$, Eq. (E-24) becomes

$$f=6\left(\frac{Dt}{a^2}\right)^{1/2}\left[\pi^{-1/2}+2\sum_{n=1}^{\infty}\operatorname{ierfc}\frac{na}{(Dt)^{1/2}}\right]-3\left(\frac{Dt}{a^2}\right)\,,\tag{E-25}$$

which may be recognized as Eq. (B-8).

E.3. Conversion to Dimensionless Form

If the definitions (D-30) and (D-31) are now utilized, along with Eq. (D-32), then Eq. (E-13) becomes

$$
\begin{aligned}
C\left(\frac{r}{a},\tau\right) = C_o &- \frac{C_o}{2(r/a)}\left[\mathrm{erfc}\,\frac{1-r/a}{2\tau^{1/2}} - \mathrm{erfc}\,\frac{1+r/a}{2\tau^{1/2}}\right] \\
&- \frac{C_o}{2(r/a)}\sum_{n=1}^{\infty}\exp\{-n\beta[n(1-\beta\tau)-r/a]\}\left[\mathrm{erfc}\,\frac{2n(1-\beta\tau)+1-r/a}{2\tau^{1/2}}\right. \\
&\qquad\left.+\mathrm{erfc}\,\frac{2n(1-\beta\tau)-1-r/a}{2\tau^{1/2}}\right] \\
&+ \frac{C_o}{2(r/a)}\sum_{n=1}^{\infty}\exp\{-n\beta[n(1-\beta\tau)+r/a]\}\left[\mathrm{erfc}\,\frac{2n(1-\beta\tau)+1+r/a}{2\tau^{1/2}}\right. \\
&\qquad\left.+\mathrm{erfc}\,\frac{2n(1-\beta\tau)-1+r/a}{2\tau^{1/2}}\right] \\
&- \frac{C_o}{(r/a)}\tau^{1/2}\left[i\mathrm{erfc}\,\frac{1-r/a}{2\tau^{1/2}} - i\mathrm{erfc}\,\frac{1+r/a}{2\tau^{1/2}}\right] \qquad \text{(E-26)} \\
&- \frac{C_o\tau^{1/2}}{(r/a)}\sum_{n=1}^{\infty}\exp\{-n\beta[n(1-\beta\tau)-r/a]\}\left[i\mathrm{erfc}\,\frac{2n(1-\beta\tau)+1-r/a}{2\tau^{1/2}}\right. \\
&\qquad\left.-i\mathrm{erfc}\,\frac{2n(1-\beta\tau)-1-r/a}{2\tau^{1/2}}\right] \\
&+ \frac{C_o\tau^{1/2}}{(r/a)}\sum_{n=1}^{\infty}\exp\{-n\beta[n(1-\beta\tau)+r/a]\}\left[i\mathrm{erfc}\,\frac{2n(1-\beta\tau)+1+r/a}{2\tau^{1/2}}\right. \\
&\qquad\left.-i\mathrm{erfc}\,\frac{2n(1-\beta\tau)-1+r/a}{2\tau^{1/2}}\right].
\end{aligned}
$$

Equation (E-21) becomes

$$
\begin{aligned}
f = 3\beta\tau &- 3(\beta\tau)^2 + (\beta\tau)^3 + 3\tau^{1/2}(1-\beta\tau)\left(i\mathrm{erfc}\,\frac{\beta\tau}{2\tau^{1/2}} + i\mathrm{erfc}\,\frac{2-\beta\tau}{2\tau^{1/2}}\right) \\
&- 12\tau^{3/2}\left(i^3\mathrm{erfc}\,\frac{\beta\tau}{2\tau^{1/2}} - i^3\mathrm{erfc}\,\frac{2-\beta\tau}{2\tau^{1/2}}\right) - 6\tau\left(i^2\mathrm{erfc}\,\frac{\beta\tau}{2\tau^{1/2}}\right. \\
&\left.- i^2\mathrm{erfc}\,\frac{2-\beta\tau}{2\tau^{1/2}}\right) + 6\tau(1-\beta\tau)\left(i^2\mathrm{erfc}\,\frac{\beta\tau}{2\tau^{1/2}} + i^2\mathrm{erfc}\,\frac{2-\beta\tau}{2\tau^{1/2}}\right) \\
&+ 3\tau^{1/2}(1-\beta\tau)\sum_{n,m=1}^{\infty}(-1)^{m+1}(2n\beta\tau^{1/2})^{m-1}\exp[-n\beta(n-1)(1-\beta\tau)]\left[i^m\mathrm{erfc}\,\frac{(2n-1)(1-\beta\tau)+1}{2\tau^{1/2}}\right. \\
&\qquad\left.+ i^m\mathrm{erfc}\,\frac{(2n-1)(1-\beta\tau)-1}{2\tau^{1/2}}\right] +
\end{aligned}
$$

$$\begin{aligned}
&+3\tau^{1/2}(1-\beta\tau)\sum_{n,m=1}^{\infty}(-1)^{m+1}(2n\beta\tau^{1/2})^{m-1}\exp[-n\beta(n+1)(1-\beta\tau)]\Big[i^m\operatorname{erfc}\frac{(2n+1)(1-\beta\tau)+1}{2\tau^{1/2}} \\
&\qquad\qquad + i^m\operatorname{erfc}\frac{(2n+1)(1-\beta\tau)-1}{2\tau^{1/2}}\Big] \\
&+6\tau\sum_{\substack{n=1\\m=2}}^{\infty}(-1)^{m+1}(m-1)(2n\beta\tau^{1/2})^{m-2}\exp[-n\beta(n-1)(1-\beta\tau)]\Big[i^m\operatorname{erfc}\frac{(2n-1)(1-\beta\tau)+1}{2\tau^{1/2}} \\
&\qquad\qquad + i^m\operatorname{erfc}\frac{(2n-1)(1-\beta\tau)-1}{2\tau^{1/2}}\Big] \\
&-6\tau\sum_{\substack{n=1\\m=2}}^{\infty}(-1)^{m+1}(m-1)(2n\beta\tau^{1/2})^{m-2}\exp[-n\beta(n+1)(1-\beta\tau)]\Big[i^m\operatorname{erfc}\frac{(2n+1)(1-\beta\tau)+1}{2\tau^{1/2}} \\
&\qquad\qquad + i^m\operatorname{erfc}\frac{(2n+1)(1-\beta\tau)-1}{2\tau^{1/2}}\Big] \\
&+6\tau(1-\beta\tau)\sum_{\substack{n=1\\m=2}}^{\infty}(-1)^{m}(2n\beta\tau^{1/2})^{m-2}\exp[-n\beta(n-1)(1-\beta\tau)]\Big[i^m\operatorname{erfc}\frac{(2n-1)(1-\beta\tau)+1}{2\tau^{1/2}} \\
&\qquad\qquad - i^m\operatorname{erfc}\frac{(2n-1)(1-\beta\tau)-1}{2\tau^{1/2}}\Big] \\
&+6\tau(1-\beta\tau)\sum_{\substack{n=1\\m=2}}^{\infty}(-1)^{m}(2n\beta\tau^{1/2})^{m-2}\exp[-n\beta(n+1)(1-\beta\tau)]\Big[i^m\operatorname{erfc}\frac{(2n+1)(1-\beta\tau)+1}{2\tau^{1/2}} \\
&\qquad\qquad - i^m\operatorname{erfc}\frac{(2n+1)(1-\beta\tau)-1}{2\tau^{1/2}}\Big] \\
&+12\tau^{3/2}\sum_{\substack{n=1\\m=3}}^{\infty}(-1)^{m}(m-2)(2n\beta\tau^{1/2})^{m-3}\exp[-n\beta(n-1)(1-\beta\tau)]\Big[i^m\operatorname{erfc}\frac{(2n-1)(1-\beta\tau)+1}{2\tau^{1/2}} \\
&\qquad\qquad - i^m\operatorname{erfc}\frac{(2n-1)(1-\beta\tau)-1}{2\tau^{1/2}}\Big] \\
&-12\tau^{3/2}\sum_{\substack{n=1\\m=3}}^{\infty}(-1)^{m}(m-2)(2n\beta\tau^{1/2})^{m-3}\exp[-n\beta(n+1)(1-\beta\tau)]\Big[i^m\operatorname{erfc}\frac{(2n+1)(1-\beta\tau)+1}{2\tau^{1/2}} \\
&\qquad\qquad - i^m\operatorname{erfc}\frac{(2n+1)(1-\beta\tau)-1}{2\tau^{1/2}}\Big],
\end{aligned} \tag{E-27}$$

and Eq. (E-25) becomes

$$f = 6\tau^{1/2}\Big[\pi^{-1/2} + 2\sum_{n=1}^{\infty} i\operatorname{erfc}\frac{n}{\tau^{1/2}}\Big] - 3\tau\,. \tag{E-28}$$

E.4. Approximate Solution for the Fractional Release

Now, if the restrictions $\frac{Dt}{a^2} < 0.01$ and $\beta\tau < 0.5$ are made, then Eq. (E-27) may be closely approximated by

$$f = 3\beta\tau - 3(\beta\tau)^2 + (\beta\tau)^3 + 3\tau^{1/2}(1-\beta\tau)\, i\operatorname{erfc}\frac{\beta\tau}{2\tau^{1/2}} -$$

$$
\begin{aligned}
&-6\tau\, i^2\mathrm{erfc}\,\frac{\beta\tau}{2\tau^{1/2}}+6\tau(1-\beta\tau)\, i^2\mathrm{erfc}\,\frac{\beta\tau}{2\tau^{1/2}}-12\tau^{3/2} i^3\mathrm{erfc}\,\frac{\beta\tau}{2\tau^{1/2}}\\
&+3\tau^{1/2}(1-\beta\tau)\sum_{n,m=1}^{\infty}(-1)^{m+1}(2n\beta\tau^{1/2})^{m-1}\exp[-n\beta(n-1)(1-\beta\tau)]\, i^m\mathrm{erfc}\,\frac{(2n-1)(1-\beta\tau)-1}{2\tau^{1/2}}\\
&+6\tau\sum_{\substack{n=1\\m=2}}^{\infty}(-1)^{m+1}(m-1)(2n\beta\tau^{1/2})^{m-2}\exp[-n\beta(n-1)(1-\beta\tau)]\, i^m\mathrm{erfc}\,\frac{(2n-1)(1-\beta\tau)-1}{2\tau^{1/2}}\\
&-6\tau(1-\beta\tau)\sum_{\substack{n=1\\m=2}}^{\infty}(-1)^{m}(2n\beta\tau^{1/2})^{m-2}\exp[-n\beta(n-1)(1-\beta\tau)]\, i^m\mathrm{erfc}\,\frac{(2n-1)(1-\beta\tau)-1}{2\tau^{1/2}}\\
&-12\tau^{3/2}\sum_{\substack{n=1\\m=3}}^{\infty}(-1)^{m}(m-2)(2n\beta\tau^{1/2})^{m-3}\exp[-n\beta(n-1)(1-\beta\tau)]\, i^m\mathrm{erfc}\,\frac{(2n-1)(1-\beta\tau)-1}{2\tau^{1/2}},
\end{aligned}
\tag{E-29}
$$

of which the $n = 1$ term is most significant.

Thus,

$$
\begin{aligned}
f=\;&3\beta\tau-3(\beta\tau)^2+(\beta\tau)^3+3\tau^{1/2}(1-\beta\tau)\, i\,\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2}\\
&-6\tau\, i^2\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2}+6\tau(1-\beta\tau)\, i^2\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2}-12\tau^{3/2} i^3\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2}\\
&+3\tau^{1/2}(1-\beta\tau)\sum_{m=1}^{\infty}(-1)^{m+1}(4)^{m-1}\left(\frac{\beta\tau^{1/2}}{2}\right)^{m-1} i^m\mathrm{erfc}\,\frac{-\beta\tau^{1/2}}{2}\\
&+6\tau\sum_{m=2}^{\infty}(-1)^{m+1}(m-1)(4)^{m-2}\left(\frac{\beta\tau^{1/2}}{2}\right)^{m-2} i^m\mathrm{erfc}\,\frac{-\beta\tau^{1/2}}{2}\\
&-6\tau(1-\beta\tau)\sum_{m=2}^{\infty}(-1)^{m}(4)^{m-2}\left(\frac{\beta\tau^{1/2}}{2}\right)^{m-2} i^m\mathrm{erfc}\,\frac{-\beta\tau^{1/2}}{2}\\
&-12\tau^{3/2}\sum_{m=3}^{\infty}(-1)^{m}(m-2)(4)^{m-3}\left(\frac{\beta\tau^{1/2}}{2}\right)^{m-3} i^m\mathrm{erfc}\,\frac{-\beta\tau^{1/2}}{2}\,.
\end{aligned}
\tag{E-30}
$$

Application of the inversion formulae for $i^m\mathrm{erfc}(-x)$--developed in Appendix C--to Eq. (E-30), upon expansion to a sufficient number of terms, reveals that terms in $\left(\frac{\beta\tau^{1/2}}{2}\right)^x$ cancel each other. Thereupon the approximate expression for the fractional release will reduce to

$$\begin{aligned} f = {} & 3\beta\tau - 3(\beta\tau)^2 + (\beta\tau)^3 - 3\tau(1-\beta\tau) - 3\tau \\ & + 6\tau^{1/2}(1-\beta\tau)\,i\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2} + 12\tau(1-\beta\tau)\,i^2\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2} \\ & + 3\tau^{1/2}(1-\beta\tau)\sum_{m=1}^{\infty}(4)^m\left(\frac{\beta\tau^{1/2}}{2}\right)^m i^{m+1}\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2} \\ & + 6\tau(1-\beta\tau)\sum_{m=1}^{\infty}(4)^m\left(\frac{\beta\tau^{1/2}}{2}\right)^m i^{m+2}\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2} \\ & + 6\tau\sum_{m=1}^{\infty}(m+1)(4)^m\left(\frac{\beta\tau^{1/2}}{2}\right)^m i^{m+2}\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2} \\ & + 12\tau^{3/2}\sum_{m=1}^{\infty}(m+1)(4)^m\left(\frac{\beta\tau^{1/2}}{2}\right)^m i^{m+3}\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2}. \end{aligned} \tag{E-31}$$

In general, the last three summations of Eq. (E-31) may be neglected in comparison with the remaining terms

$$\begin{aligned} f = {} & 3\beta\tau(1-\beta\tau) + (\beta\tau)^3 - 3\tau - 3\tau(1-\beta\tau) \\ & + 6\tau^{1/2}(1-\beta\tau)\,i\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2} + 12\tau(1-\beta\tau)\,i^2\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2} \\ & + 3\tau^{1/2}(1-\beta\tau)\sum_{m=1}^{\infty}(4)^m\left(\frac{\beta\tau^{1/2}}{2}\right)^m i^{m+1}\mathrm{erfc}\,\frac{\beta\tau^{1/2}}{2}. \end{aligned} \tag{E-32}$$

NOMENCLATURE

a	Characteristic dimension at initial conditions; half thickness for a slab; radius for a sphere (cm)
b	Rate of boundary movement (cm/sec)
C	Concentration of the tracer element (atoms/cm^3)
C_0	Initial concentration of the tracer (atoms/cm^3)
D	Diffusion coefficient for the tracer atoms (cm^2/sec)
f	Fractional release of the tracer element
Q	Number of tracer atoms
Q_0	Initial value of Q
r	Space coordinate in spherical geometry (cm)
t	Time from start of evaporation/diffusion (sec)
x	Space coordinate in slab geometry (cm)
β	Dimensionless evaporation/diffusion coefficient [Eq. (II-8)]
ξ	Integration variable (cm)
τ	Dimensionless time [Eq. (II-7)]

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